

WEST Search History

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DATE: Wednesday, December 12, 2007

| Hide? | Set Name | Query | Hit Count |
|--------------------------|----------|--|-----------|
| | | <i>DB=PGPB,USPT; PLUR=YES; OP=ADJ</i> | |
| <input type="checkbox"/> | L4 | (pyrrolo adj3 pyridazine) | 8 |
| <input type="checkbox"/> | L3 | L2 and (pyrrolo adj3 pyridazine) | 0 |
| <input type="checkbox"/> | L2 | 514/525.06.icls. or 514/252.06.ccls. or 544/236.icls. or 544/236.ccls. | 910 |
| <input type="checkbox"/> | L1 | 6342601.pn. | 1 |

END OF SEARCH HISTORY

FILE 'REGISTRY' ENTERED AT 10:19:12 ON 12 DEC 2007
L1 STRUCTURE UPLOADED
L2 0 S L1
L3 237 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 10:21:22 ON 12 DEC 2007
L4 7 S L3

FILE 'REGISTRY' ENTERED AT 10:28:45 ON 12 DEC 2007
L5 STRUCTURE UPLOADED
L6 1 S L5
L7 86 S L5 SSS FULL

FILE 'CAPLUS' ENTERED AT 10:29:37 ON 12 DEC 2007
L8 19 S L7
L9 18 S L8 NOT L4

FILE 'REGISTRY' ENTERED AT 11:33:03 ON 12 DEC 2007
L10 STRUCTURE UPLOADED
L11 3 S L10
L12 54 S L10 SSS FULL

FILE 'CAPLUS' ENTERED AT 11:36:06 ON 12 DEC 2007
L13 4 S L12

=> file registry
COST IN U.S. DOLLARS

| SINCE FILE | TOTAL |
|------------|---------|
| ENTRY | SESSION |
| 0.21 | 0.21 |

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 10:19:12 ON 12 DEC 2007
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 11 DEC 2007 HIGHEST RN 957570-32-0
DICTIONARY FILE UPDATES: 11 DEC 2007 HIGHEST RN 957570-32-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

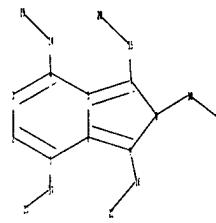
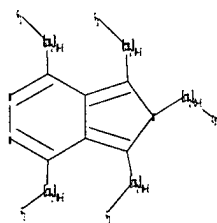
TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>
Uploading C:\Program Files\Stnexp\Queries\10520962broad.str



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10 11 14 15 16 17 19 20 22 23
ring nodes :
1 2 3 4 5 6 7 8 9
chain bonds :
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ring bonds :
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exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 10-11 14-19 15-20 16-22 17-23

exact bonds :
1-17 4-14 7-15 8-10 9-16

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G1:H,Cy

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Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:Atom 14:CLASS 15:CLASS 16:CLASS 17:CLASS 19:CLASS 20:CLASS 22:CLASS
23:CLASS

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L1 STRUCTURE UPLOADED

=> s l1

SAMPLE SEARCH INITIATED 10:19:30 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 78197 TO ITERATE

2.6% PROCESSED 2000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**

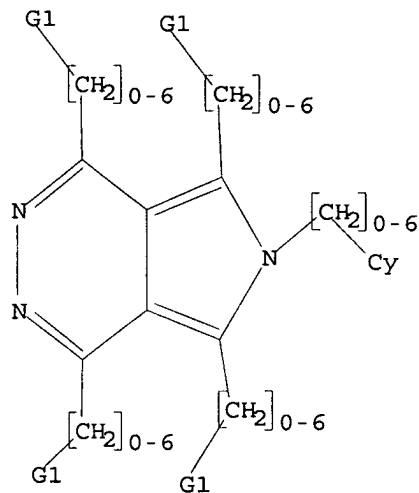
PROJECTED ITERATIONS: 1547303 TO 1580577
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> d l1

L1 HAS NO ANSWERS

L1 STR



G1 H,Cy

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss full

FULL SEARCH INITIATED 10:19:58 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1557677 TO ITERATE

64.2% PROCESSED 1000000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.16

237 ANSWERS

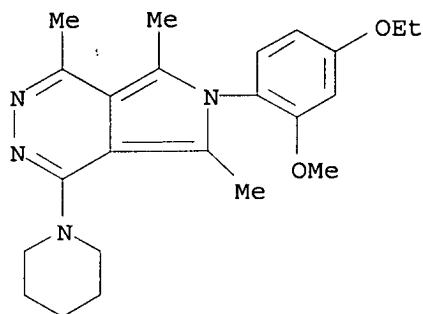
FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**

PROJECTED ITERATIONS: 1557677 TO 1557677
PROJECTED ANSWERS: 312 TO 426

L3 237 SEA SSS FUL L1

=> d 13 scan

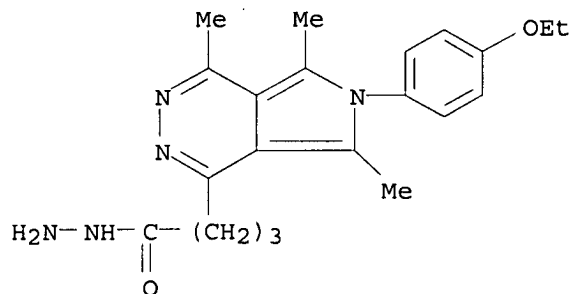
L3 237 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 6H-Pyrrolo[3,4-d]pyridazine, 6-(4-ethoxy-2-methoxyphenyl)-1,5,7-trimethyl-
4-(1-piperidinyl)-
MF C23 H30 N4 O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

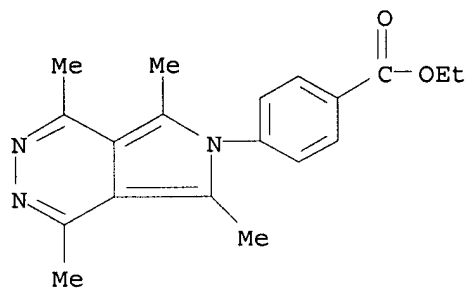
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

L3 237 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 6H-Pyrrolo[3,4-d]pyridazine-1-butanoic acid, 6-(4-ethoxyphenyl)-4,5,7-
trimethyl-, hydrazide
MF C21 H27 N5 O2



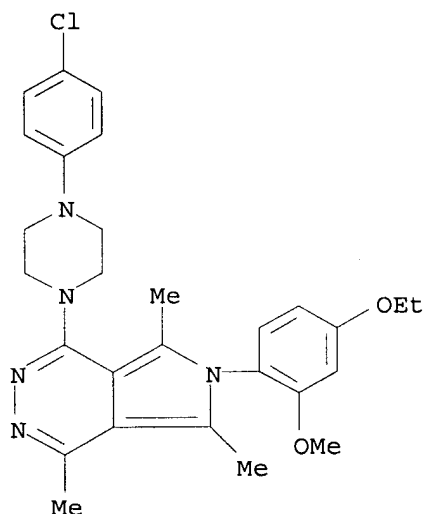
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 237 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Benzoic acid, 4-(1,4,5,7-tetramethyl-6H-pyrrolo[3,4-d]pyridazin-6-yl)-, ethyl ester
MF C19 H21 N3 O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 237 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
 IN 6H-Pyrrolo[3,4-d]pyridazine, 1-[4-(4-chlorophenyl)-1-piperazinyl]-6-(4-ethoxy-2-methoxyphenyl)-4,5,7-trimethyl-
 MF C28 H32 Cl N5 O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE
ENTRY
173.45

TOTAL
SESSION
173.66

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 10:21:22 ON 12 DEC 2007

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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FILE COVERS 1907 - 12 Dec 2007 VOL 147 ISS 25
FILE LAST UPDATED: 11 Dec 2007 (20071211/ED)

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<http://www.cas.org/infopolicy.html>

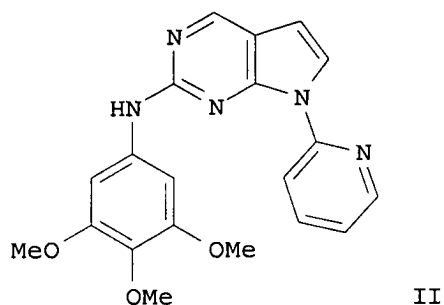
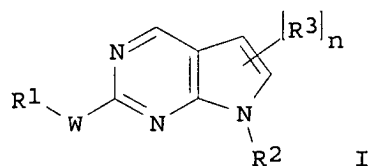
=> s l3

L4 7 L3

=> d l4 1-7 ti abs bib

L4 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN
TI Expedited SAR study of high-affinity ligands to the $\alpha 2\delta$
subunit of voltage-gated calcium channels: Generation of a focused library
using a solution-phase Sn2Ar coupling methodology
AB The SAR of the lead compound 3, a novel ligand for the $\alpha 2\delta$
subunit of voltage-gated calcium channels, was rapidly explored.
Utilizing a parallel solution-phase Sn2Ar coupling approach, a focused
library was obtained. The library was evaluated in vitro and afforded a
series of analogs with improved potencies. The SAR trends of the library
are also described.
AN 2005:1342000 CAPLUS <<LOGINID::20071212>>
DN 144:100381
TI Expedited SAR study of high-affinity ligands to the $\alpha 2\delta$
subunit of voltage-gated calcium channels: Generation of a focused library
using a solution-phase Sn2Ar coupling methodology
AU Chen, Chixu; Stearns, Brian; Hu, Tao; Anker, Naomi; Santini, Angelina;
Arruda, Jeannie M.; Campbell, Brian T.; Datta, Purabi; Aiyar, Jayashree;
Munoz, Benitio
CS Department of Chemistry, Merck Research Laboratories, San Diego, CA,
92121, USA
SO Bioorganic & Medicinal Chemistry Letters (2006), 16(3), 746-749
CODEN: BMCLE8; ISSN: 0960-894X
PB Elsevier B.V.
DT Journal
LA English
OS CASREACT 144:100381
RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN
TI Preparation of substituted pyrrolo[2,3-d]pyrimidines as inducers of
keratinocyte differentiation
GI



AB The invention provides compds. I [$n = 0-2$; $W = \text{NR}_4, \text{S}, \text{O}, \text{SO}, \text{SO}_2$ (wherein $\text{R}_4 = \text{H}, \text{alkyl}$); $\text{R}_1 = \text{arylalkyl}, \text{heteroarylalkyl}, \text{cycloalkylalkyl}, \text{etc.}$; $\text{R}_2 = \text{arylalkyl}, \text{heteroarylalkyl}, \text{cycloalkylalkyl}, \text{etc.}$; $\text{R}_3 = \text{halo}, \text{OH}, \text{XSR}_5, \text{etc.}$ ($\text{X} = \text{a bond}, \text{alkylene}$; $\text{R}_5 = \text{H}, \text{alkyl}, \text{cycloalkylalkyl}$)], pharmaceutical compns. comprising such compds. and methods of using such compds. to induce undifferentiated keratinocytes to differentiate into terminally differentiated keratinocytes. The invention further provides compds. for the treatment of diseases or disorders associated with casein kinase II (CK2), TANK-binding kinase 1 (TBK1) and NIMA-related kinase 9 (NEK9). Over 200 compds. I were prepared E.g., a 4-step synthesis of II, starting from 5-bromo-2,4-dichloropyrimidine, was given.

AN 2005:1220346 CAPLUS <<LOGINID::20071212>>

DN 143:477978

TI Preparation of substituted pyrrolo[2,3-d]pyrimidines as inducers of keratinocyte differentiation

IN Hong, Jiyong; Gray, Nathanael S.; Schultz, Peter

PA IRM LLC, Bermuda

SO PCT Int. Appl., 53 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|----|--|------|----------|-----------------|----------|
| PI | WO 2005107760 | A1 | 20051117 | WO 2005-US15118 | 20050429 |
| | W: | | | | |
| | AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| | RW: | | | | |
| | BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |

PRAI US 2004-567346P P 20040430

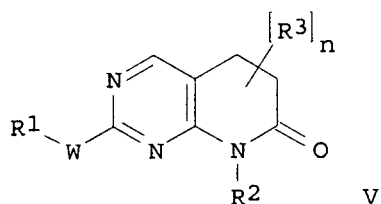
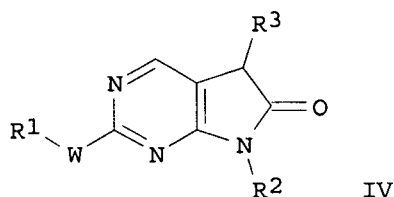
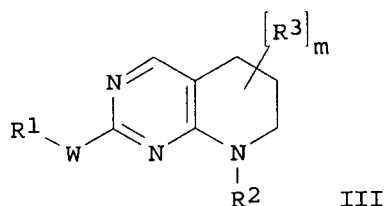
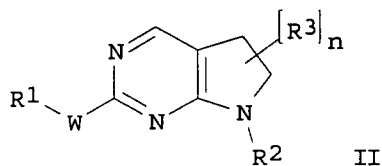
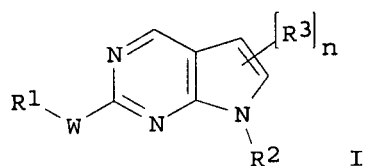
OS CASREACT 143:477978; MARPAT 143:477978

RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN

TI Preparation of pyrrolopyrimidines and their analogs as protein kinase inhibitors

GI



AB The invention provides a novel class of compds. I-V [n = 0-2; m = 0-3; W = NR₄, S, O, SO, SO₂ (wherein R₄ = H, alkyl); R₁ = (un)substituted (hetero)arylalkyl, (hetero)cycloalkyl; R₂ = (un)substituted (hetero)arylalkyl, (hetero)cycloalkyl; R₃ = halo, OH, XSR₅, etc. (X = a bond, alkylene; R₅ = H, alkyl, cycloalkylalkyl)], pharmaceutical compns. comprising such compds. and methods of using such compds. to treat or prevent diseases or disorders associated with abnormal or deregulated kinase activity, particularly diseases or disorders that involve abnormal activation of the FAK, Abl, BCR-Abl, PDGF-R, c-Kit, NPM-ALK, Flt-3, JAK2 and c-Met kinases. Over 200 compds. I-V were prepared and characterized. The preparation of the compds. I is illustrated in examples. E.g., synthesis of I [R₁ = 3,4,6-(MeO)₃C₆H₂; R₂ = 2-pyridyl; R₃ = H; W = NH], starting from 5-bromo-2,4-dichloropyrimidine, was given. The compds. I-V were tested against various kinases. For example, they inhibit the enzyme activity by 50% (IC₅₀), in a concentration of from 0.001 to 0.5 μM,

especially from

0.01 to 0.1 μM.

AN 2005:962258 CAPLUS <<LOGINID::20071212>>

DN 143:266947

TI Preparation of pyrrolopyrimidines and their analogs as protein kinase inhibitors

IN Choi, Ha-Soon; Wang, Zhicheng; Gray, Nathanael Schiander; Gu, Xiang-Ju; He, Xiaohui; He, Yun; Jiang, Tao; Liu, Yi; Richmond, Wendy; Sim, Taebo; Yang, Kunyong

PA IRM LLC, Bermuda

SO PCT Int. Appl., 63 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------|------|----------|-----------------|----------|
| PI WO 2005080393 | A1 | 20050901 | WO 2005-US4630 | 20050214 |

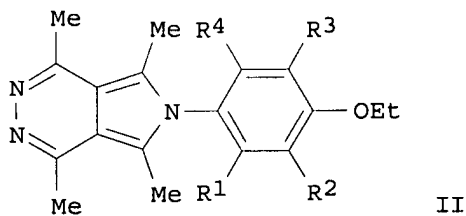
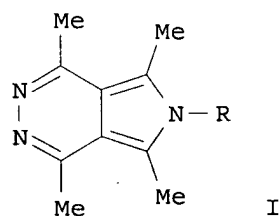
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| | | | | |
|---|----|----------|------------------|----------|
| AU 2005214352 | A1 | 20050901 | AU 2005-214352 | 20050214 |
| CA 2553785 | A1 | 20050901 | CA 2005-2553785 | 20050214 |
| EP 1713806 | A1 | 20061025 | EP 2005-713510 | 20050214 |
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| CN 1918158 | A | 20070221 | CN 2005-80004895 | 20050214 |
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| JP 2007522241 | T | 20070809 | JP 2006-553321 | 20050214 |
| MX 2006PA09158 | A | 20061110 | MX 2006-PA9158 | 20060811 |
| IN 2006CN02987 | A | 20070608 | IN 2006-CN2987 | 20060814 |
| US 2007225306 | A1 | 20070927 | US 2007-589099 | 20070611 |
| PRAI US 2004-544944P | P | 20040214 | | |
| WO 2005-US4630 | W | 20050214 | | |

OS MARPAT 143:266947

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

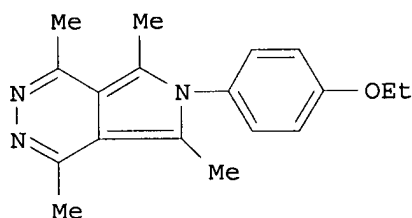
L4 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN
 TI Synthesis and biological evaluation of 6-aryl-6H-pyrrolo[3,4-d]pyridazine derivatives as high-affinity ligands of the $\alpha 2\delta$ subunit of voltage-gated calcium channels
 GI



AB 2H-pyrrolo[3,4-c]pyridazines I (R = 4-EtOC6H4, 2-EtO-5-pyridinyl, 5-EtO-2-pyridinyl, 5-EtO-2-pyrazinyl, 4-EtO-1-pyridazinyl, 2-EtO-5-pyrimidinyl, etc.) such as II (R1 = H, MeO, Et, H2C:CH, Me, MeS, EtO, F; R2 = H, Me; R3 = H, Me, Cl, HOCH2; R4 = H, Me) are prepared as ligands for the $\alpha 2\delta$ subunit of voltage-gated calcium channels. Ortho-substituents capable of electron-donation increase the binding of II to the $\alpha 2\delta$ subunit of voltage-gated calcium channels; electron-withdrawing substituents in the ortho-position of II decrease binding significantly. II (R1 = MeO; R2 = R3 = R4 = H) binds to the $\alpha 2\delta$ subunit of voltage-gated calcium channels from A710 cells with an IC50 value of 4 nM. Testing of tritiated ligand II (R1 = TCH2TCH; R2 = R3 = R4 = H) in purified human $\alpha 2\delta$ voltage-gated calcium channel subunits indicates that II displace Gabapentin from the $\alpha 2\delta$ subunit of voltage-gated calcium channels, and thus act as Gabapentin mimics in vitro. In the preparation of II (R1 = Et; R2 = R3 = R4 = H), a novel metal-free hydrogenation is used using hydrazine as the reductant; the reduction is effective in other systems (no data).

AN 2004:303255 CAPLUS <<LOGINID::20071212>>
 DN 141:54277
 TI Synthesis and biological evaluation of 6-aryl-6H-pyrrolo[3,4-d]pyridazine derivatives as high-affinity ligands of the $\alpha 2\delta$ subunit of voltage-gated calcium channels
 AU Hu, Tao; Stearns, Brian A.; Campbell, Brian T.; Arruda, Jeannie M.; Chen, Chixu; Aiyar, Jayashree; Bezverkov, Robert E.; Santini, Angelina; Schaffhauser, Herve; Liu, Wensheng; Venkatraman, Shankar; Munoz, Benito
 CS MRLSDB2, Department of Medicinal Chemistry, Merck Research Laboratories, San Diego, CA, 92121, USA
 SO Bioorganic & Medicinal Chemistry Letters (2004), 14(9), 2031-2034
 CODEN: BMCLE8; ISSN: 0960-894X
 PB Elsevier Science B.V.
 DT Journal
 LA English
 OS CASREACT 141:54277
 RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN
 TI Synthesis and biological evaluation of 6-aryl-6H-pyrrolo[3,4-d]pyridazine derivatives: high-affinity ligands to the $\alpha 2\delta$ subunit of voltage gated calcium channels
 GI



AB A novel class of 6-aryl-6H-pyrrolo[3,4-d]pyridazine ligands for the $\alpha 2\delta$ subunit of voltage-gated calcium channels has been described. Substitutions in the aryl ring of the mol. were generally not tolerated, and resulted in diminished binding to the $\alpha 2\delta$ subunit. Modifications to the pyridazine ring revealed numerous permissive substitutions, and detailed SAR studies were carried out in this portion of the mol. Replacement of the pyridazine ring Me group with an aminomethyl functionality provided greatly improved potency over the initial lead. The initial lead compound (I) displayed good rat pharmacokinetic properties, and was shown to be efficacious in the Chung model for neuropathic pain in rats.

AN 2004:153601 CAPLUS <<LOGINID::20071212>>
 DN 140:357282
 TI Synthesis and biological evaluation of 6-aryl-6H-pyrrolo[3,4-d]pyridazine derivatives: high-affinity ligands to the $\alpha 2\delta$ subunit of voltage gated calcium channels
 AU Stearns, Brian A.; Anker, Naomi; Arruda, Jeannie M.; Campbell, Brian T.; Chen, Chixu; Cramer, Merryl; Hu, Tao; Jiang, Xiaohui; Park, Kenneth; Ren, Kun Kun; Sablad, Marciano; Santini, Angelina; Schaffhauser, Herve; Urban, Mark O.; Munoz, Benito
 CS Department of Medicinal Chemistry, Merck Research Laboratories, San Diego, CA, 92121, USA
 SO Bioorganic & Medicinal Chemistry Letters (2004), 14(5), 1295-1298
 CODEN: BMCLE8; ISSN: 0960-894X

PB Elsevier Science B.V.

DT Journal

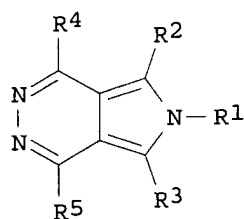
LA English

OS CASREACT 140:357282

RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN

TI Treatment of neuropathic pain with 6H-pyrrolo[3,4-d]pyridazine compounds
GI



AB The title compds. [I; R1 = (un)substituted alkyl(hetero)aryl, alkyl(hetero)cycloalkyl, (hetero)aryl, (hetero)cycloalkyl; R2-R5 = a bond, (un)substituted alkyl, alkyl(hetero)aryl, alkyl(hetero)cycloalkyl, (hetero)aryl, (hetero)cycloalkyl] were prepared as as ligands of voltage gated calcium channels (VGCC), useful in the treatment of neuropathic pain, and psychiatric and mood disorders such as, for example, schizophrenia, anxiety, depression, panic, and bipolar disorder, as well as in the treatment of pain, Parkinson s disease, cognitive dysfunction, epilepsy, circadian rhythm disorders, drug addiction, drug abuse, drug withdrawal and other. E.g., a multi-step synthesis of I [R1 = 4-EtOC6H4; R2-R4 = Me; R5 = 4-MeOC6H4] which produced a 65% effect after i.p. dosing at 30 mg/kg in spinal nerve ligation model of neuropathic pain in rats, was given. The pharmaceutical composition comprising the compound I is claimed.

AN 2004:60243 CAPLUS <<LOGINID::20071212>>

DN 140:111422

TI Treatment of neuropathic pain with 6H-pyrrolo[3,4-d]pyridazine compounds

IN Anker, Naomi Burke; Arruda, Jeannie M.; Campbell, Brian Thomas; Munoz, Benito; Prasit, Petpiboon; Stearns, Brian A.

PA Merck & Co., Inc., USA

SO PCT Int. Appl., 203 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|----|--|------|----------|-----------------|----------|
| PI | WO 2004006836 | A2 | 20040122 | WO 2003-US21493 | 20030708 |
| | WO 2004006836 | A3 | 20040415 | | |
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| | RW: | | | | |
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| | CA 2492022 | A1 | 20040122 | CA 2003-2492022 | 20030708 |

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| EP 1539168 | A2 | 20050615 | EP 2003-764414 | 20030708 |
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| JP 2005536507 | T | 20051202 | JP 2004-521592 | 20030708 |
| US 2006154929 | A1 | 20060713 | US 2005-520962 | 20051128 |
| PRAI US 2002-394734P | P | 20020711 | | |
| WO 2003-US21493 | W | 20030708 | | |
| OS | MARPAT 140:111422 | | | |

L4 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN
 TI Synthesis and electrophilic substitution of dipyrrolo[1,2-b:3,4-d]pyridazines
 AB Dipyrrolo[1,2-b:3,4-d]pyridazines were prepared from 1,4,5,7-tetramethyl-6-R1-pyrrolo[3,4-d]-pyridazines. The dipyrrolo[1,2-b:3,4-d]pyridazines were found to have high nucleophilicity and electrophilic substitution occurs at C7, or C7 and C9 depending on the steric bulk and activity of the attacking electrophile.
 AN 2003:927977 CAPLUS <<LOGINID::20071212>>
 DN 140:303615
 TI Synthesis and electrophilic substitution of dipyrrolo[1,2-b:3,4-d]pyridazines
 AU Arsen'ev, V. G.; Arsen'eva, M. Yu.; Shopin, D. V.; Olekhovich, L. P.
 CS Rostov State University, Rostov-on-Don, 344006, Russia
 SO Chemistry of Heterocyclic Compounds (New York, NY, United States) (Translation of Khimiya Geterotsiklicheskich Soedinenii) (2003), 39(5), 669-670
 CODEN: CHCCAL; ISSN: 0009-3122
 PB Kluwer Academic/Consultants Bureau
 DT Journal
 LA English
 OS CASREACT 140:303615
 RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

(FILE 'HOME' ENTERED AT 10:19:03 ON 12 DEC 2007)

FILE 'REGISTRY' ENTERED AT 10:19:12 ON 12 DEC 2007

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|----|--------------------|
| L1 | STRUCTURE UPLOADED |
| L2 | 0 S L1 |
| L3 | 237 S L1 SSS FULL |

FILE 'CAPLUS' ENTERED AT 10:21:22 ON 12 DEC 2007

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| L4 | 7 S L3 |
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| FULL ESTIMATED COST | 20.28 | 193.94 |
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| CA SUBSCRIBER PRICE | -5.46 | -5.46 |

SESSION WILL BE HELD FOR 120 MINUTES
 STN INTERNATIONAL SESSION SUSPENDED AT 10:21:37 ON 12 DEC 2007

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSPTAEXO1623

PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *
SESSION RESUMED IN FILE 'CAPLUS' AT 10:28:35 ON 12 DEC 2007
FILE 'CAPLUS' ENTERED AT 10:28:35 ON 12 DEC 2007
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| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
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| CA SUBSCRIBER PRICE | -5.46 | -5.46 |

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STRUCTURE FILE UPDATES: 11 DEC 2007 HIGHEST RN 957570-32-0
DICTIONARY FILE UPDATES: 11 DEC 2007 HIGHEST RN 957570-32-0

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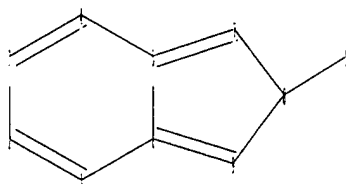
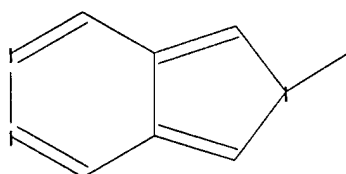
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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

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 ring nodes :
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 ring bonds :
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 1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 8-10

G1:H,Cy

Match level :
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS

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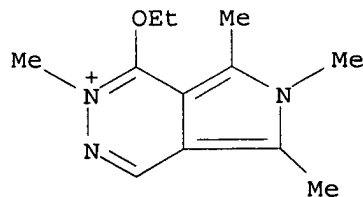
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L6 1 SEA SSS SAM L5

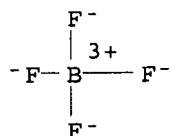
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L6 1 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
 IN 6H-Pyrrolo[3,4-d]pyridazinium, 1-ethoxy-2,5,6,7-tetramethyl-,
 tetrafluoroborate(1-) (9CI)
 MF C12 H18 N3 O . B F4

CM 1



CM 2



ALL ANSWERS HAVE BEEN SCANNED

=> s 15 sss full
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 FULL SCREEN SEARCH COMPLETED - 120189 TO ITERATE

100.0% PROCESSED 120189 ITERATIONS 86 ANSWERS
 SEARCH TIME: 00.00.01

L7 86 SEA SSS FUL L5

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|--|------------|---------|
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| | ENTRY | SESSION |
| FULL ESTIMATED COST | 172.10 | 366.04 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL |
| | ENTRY | SESSION |
| CA SUBSCRIBER PRICE | 0.00 | -5.46 |

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 FILE LAST UPDATED: 11 Dec 2007 (20071211/ED)

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<http://www.cas.org/infopolicy.html>

=> s 17
 L8 19 L7

=> d 18 1-19 ti abs bib hitstr

L8 ANSWER 1 OF 19 CAPLUS COPYRIGHT 2007 ACS on STN
 TI Synthesis of 5-aryl-2-oxopyrrole derivatives as synthons for highly substituted pyrroles
 AB A small library of 2-oxo-5-(hetero)arylpyrroles was prepared starting from 2,3-dioxo-5-(hetero)arylpyrrolidines. The large synthetic possibilities

of these 2-oxopyrroles were investigated. The 2-oxopyrroles offer a large number of possible derivatizations including reactions with electrophiles. The chloroformylation of 2-oxo-5-(hetero)arylprrroles provides pyrrole carbaldehydes. Some pyrrole carbaldehydes were used to synthesize polycyclic compds. like pyrrolo[3,4-d]pyridazinones, a thienopyrrole, a pyrrolobenz[1,4]oxazepine, a pyrrolobenzo[1,4]thiazepine, and a pyrrolobenzo[1,4]diazepine. Hereby we showed through a short exploration that the oxopyrroles and analogs are interesting and versatile synthetic building blocks.

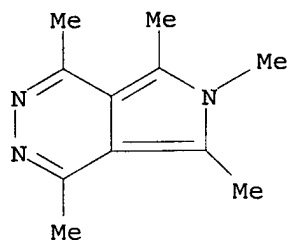
AN 2006:498781 CAPLUS <<LOGINID::20071212>>
DN 145:167033
TI Synthesis of 5-aryl-2-oxopyrrole derivatives as synthons for highly substituted pyrroles
AU Metten, Bert; Kostermans, Maarten; Van Baelen, Gitte; Smet, Mario; Dehaen, Wim
CS Department of Chemistry, Katholieke Universiteit Leuven, Louvain, B-3001, Belg.
SO Tetrahedron (2006), 62(25), 6018-6028
CODEN: TETRAB; ISSN: 0040-4020
PB Elsevier B.V.
DT Journal
LA English
OS CASREACT 145:167033
IT 901764-67-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of library of 5-aryl-2-oxopyrrole derivs. from
2,3-dioxo-5-arylprrrolidines and their use as synthons for highly
substituted pyrroles)
RN 901764-67-8 CAPLUS
CN 1H-Pyrrolo[3,4-d]pyridazin-1-one, 5-chloro-2,6-dihydro-7-phenyl-6-
(phenylmethyl)- (CA INDEX NAME)

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RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

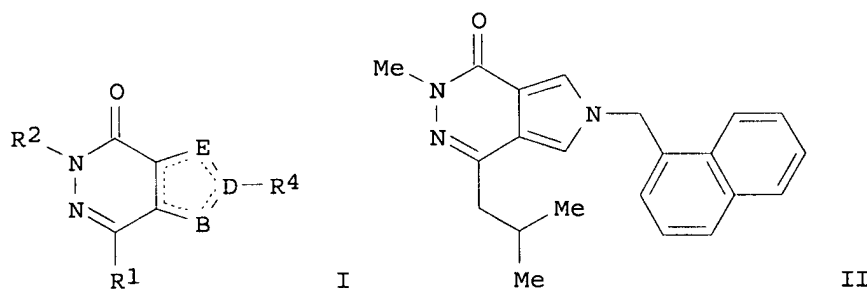
L8 ANSWER 2 OF 19 CAPLUS COPYRIGHT 2007 ACS on STN
TI Synthesis and electrophilic substitution of dipyrrolo[1,2-b:3,4-d]pyridazines
AB Dipyrrolo[1,2-b:3,4-d]pyridazines were prepared from 1,4,5,7-tetramethyl-6-R1-pyrrolo[3,4-d]-pyridazines. The dipyrrolo[1,2-b:3,4-d]pyridazines were found to have high nucleophilicity and electrophilic substitution occurs at C7, or C7 and C9 depending on the steric bulk and activity of the attacking electrophile.
AN 2003:927977 CAPLUS <<LOGINID::20071212>>
DN 140:303615
TI Synthesis and electrophilic substitution of dipyrrolo[1,2-b:3,4-d]pyridazines
AU Arsen'ev, V. G.; Arsen'eva, M. Yu.; Shopin, D. V.; Olekhovich, L. P.
CS Rostov State University, Rostov-on-Don, 344006, Russia
SO Chemistry of Heterocyclic Compounds (New York, NY, United States) (Translation of Khimiya Geterotsiklicheskich Soedinenii) (2003), 39(5), 669-670
CODEN: CHCCAL; ISSN: 0009-3122
PB Kluwer Academic/Consultants Bureau
DT Journal
LA English
OS CASREACT 140:303615
IT 79398-46-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of dipyrrolopyridazines from pyrrolopyridazines and their reactivity in electrophilic substitution reactions)

RN 79398-46-2 CAPLUS
CN 6H-Pyrrolo[3,4-d]pyridazine, 1,4,5,6,7-pentamethyl- (CA INDEX NAME)



RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 3 OF 19 CAPLUS COPYRIGHT 2007 ACS on STN
TI Preparation of novel fused pyridazinones useful as immunosuppressants
GI



AB The invention provides certain pyrrolo-, thieno-, furano- and pyrazolo[3,4-d]pyridazinones of general formula I [B = CH, N, S, or O; D = C or N; E = CR³ or N; with various dependencies; R¹ = alkyl, alkoxy, (di)(alkyl)amino, Ph, cycloalkyl, etc.; R² = Me, alkyl, alkoxyalkyl; R³ = H, (un)substituted carbamoyl, various derivs. of OH and SH; R⁴ = (un)substituted (hetero)arylmethyl, (hetero)aroyl, (hetero)arylhydroxymethyl, acenaphthenyl, indanyl, or fluorenyl] and their pharmaceutically acceptable salts or solvates. Also disclosed are processes for their preparation, pharmaceutical compns. containing them, a process

for preparing the pharmaceutical compns., and methods of treatment involving their use. In particular, their use in immunosuppression, and especially in therapy of reversible obstructive airways diseases, is claimed. For example, title compound II was prepared in 4 steps: (1) bromination of 4-methyl-2-pentanone and reaction with Ph₃P:CHCO₂Me to give (E)-Me 6-methyl-4-oxo-2-heptenoate; (2) cyclization of the latter with tosylmethyl isocyanide in DMSO to give a pyrrole derivative; (3) N-alkylation of the pyrrole using NaH and 1-naphthalenylmethyl chloride in DMF; and (4) cyclocondensation of the pyrrole sidechains with methylhydrazine. As inhibitors of human mixed lymphocyte reaction in vitro, the example compds. had IA₅₀ values of < 1 + 10⁻⁶ M.

AN 1999:388188 CAPLUS <<LOGINID::20071212>>
DN 131:44836
TI Preparation of novel fused pyridazinones useful as immunosuppressants

IN Bantick, John; Cooper, Martin; Thorne, Philip; Perry, Matthew
PA Astra Pharmaceuticals Ltd., UK; Astra Aktiebolag
SO PCT Int. Appl., 94 pp.
CODEN: PIXXD2

DT Patent
LA English

FAN.CNT 2

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
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| PI | WO 9929695 | A1 | 19990617 | WO 1998-SE2191 | 19981201 |
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| | RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
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| | AU 9917916 | A | 19990628 | AU 1999-17916 | 19981201 |
| | EP 1036076 | A1 | 20000920 | EP 1998-962754 | 19981201 |
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| | BR 9813373 | A | 20001003 | BR 1998-13373 | 19981201 |
| | TR 200001603 | T2 | 20001023 | TR 2000-1603 | 19981201 |
| | EE 200000318 | A | 20010815 | EE 2000-318 | 19981201 |
| | HU 2001000280 | A2 | 20011028 | HU 2001-280 | 19981201 |
| | HU 2001000280 | A3 | 20030328 | | |
| | JP 2001525413 | T | 20011211 | JP 2000-524288 | 19981201 |
| | NZ 504452 | A | 20020531 | NZ 1998-504452 | 19981201 |
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| | US 6342601 | B1 | 20020129 | US 1999-214755 | 19990112 |
| | NO 2000002788 | A | 20000801 | NO 2000-2788 | 20000531 |
| | US 2002099055 | A1 | 20020725 | US 2001-6244 | 20011210 |
| | US 6770646 | B2 | 20040803 | | |
| | US 2004162410 | A1 | 20040819 | US 2004-776245 | 20040212 |
| PRAI | SE 1997-4542 | A | 19971205 | | |
| | SE 1998-1989 | A | 19980604 | | |
| | GB 1995-26273 | A | 19951221 | | |
| | SE 1996-556 | A | 19960215 | | |
| | WO 1996-SE1680 | W | 19961217 | | |

=> s 18 not 14

L9 18 L8 NOT L4

=> d 19 1-18 ti abs bib hitstr

L9 ANSWER 1 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN

TI Synthesis of 5-aryl-2-oxopyrrole derivatives as synthons for highly substituted pyrroles

AB A small library of 2-oxo-5-(hetero)arylpyrroles was prepared starting from 2,3-dioxo-5-(hetero)arylpyrrolidines. The large synthetic possibilities of these 2-oxopyrroles were investigated. The 2-oxopyrroles offer a large number of possible derivatizations including reactions with electrophiles. The chloroformylation of 2-oxo-5-(hetero)arylpyrroles provides pyrrole carbaldehydes. Some pyrrole carbaldehydes were used to synthesize polycyclic compds. like pyrrolo[3,4-d]pyridazinones, a thienopyrrole, a pyrrolobenz[1,4]oxazepine, a pyrrolobenzo[1,4]thiazepine, and a pyrrolobenzo[1,4]diazepine. Hereby we showed through a short exploration that the oxopyrroles and analogs are interesting and versatile synthetic building blocks.

AN 2006:498781 CAPLUS <<LOGINID::20071212>>

DN 145:167033

TI Synthesis of 5-aryl-2-oxopyrrole derivatives as synthons for highly

substituted pyrroles

AU Metten, Bert; Kostermans, Maarten; Van Baelen, Gitte; Smet, Mario; Dehaen, Wim

CS Department of Chemistry, Katholieke Universiteit Leuven, Louvain, B-3001, Belg.

SO Tetrahedron (2006), 62(25), 6018-6028
CODEN: TETRAB; ISSN: 0040-4020

PB Elsevier B.V.

DT Journal

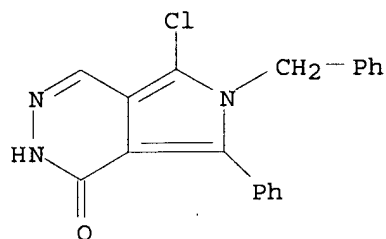
LA English

OS CASREACT 145:167033

IT 901764-67-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of library of 5-aryl-2-oxopyrrole derivs. from
2,3-dioxo-5-arylpyrrolidines and their use as synthons for highly
substituted pyrroles)

RN 901764-67-8 CAPLUS

CN 1H-Pyrrolo[3,4-d]pyridazin-1-one, 5-chloro-2,6-dihydro-7-phenyl-6-(phenylmethyl)- (CA INDEX NAME)

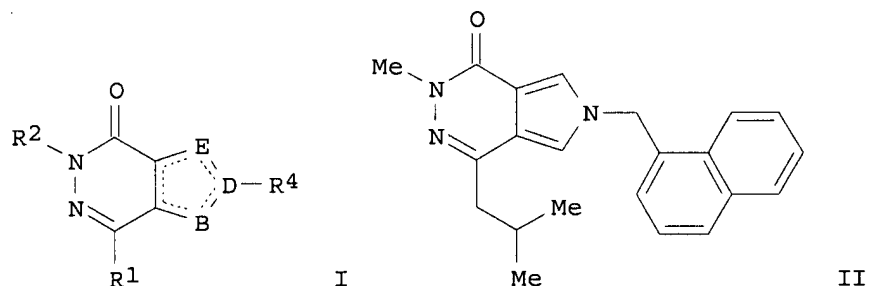


RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 2 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN

TI Preparation of novel fused pyridazinones useful as immunosuppressants

GI



AB The invention provides certain pyrrolo-, thieno-, furano- and pyrazolo[3,4-d]pyridazinones of general formula I [B = CH, N, S, or O; D = C or N; E = CR₃ or N; with various dependencies; R₁ = alkyl, alkoxy, (di)(alkyl)amino, Ph, cycloalkyl, etc.; R₂ = Me, alkyl, alkoxyalkyl; R₃ = H, (un)substituted carbamoyl, various derivs. of OH and SH; R₄ = (un)substituted (hetero)arylmethyl, (hetero)aroyl, (hetero)arylhydroxymethyl, acenaphthenyl, indanyl, or fluorenyl] and their

pharmaceutically acceptable salts or solvates. Also disclosed are processes for their preparation, pharmaceutical compns. containing them, a process

for preparing the pharmaceutical compns., and methods of treatment involving their use. In particular, their use in immunosuppression, and especially in therapy of reversible obstructive airways diseases, is claimed. For example, title compound II was prepared in 4 steps: (1) bromination of 4-methyl-2-pentanone and reaction with Ph3P:CHCO2Me to give (E)-Me 6-methyl-4-oxo-2-heptenoate; (2) cyclization of the latter with tosylmethyl isocyanide in DMSO to give a pyrrole derivative; (3) N-alkylation of the pyrrole using NaH and 1-naphthalenylmethyl chloride in DMF; and (4) cyclocondensation of the pyrrole sidechains with methylhydrazine. As inhibitors of human mixed lymphocyte reaction in vitro, the example compds. had IA50 values of $< 1 + 10^{-6}$ M.

AN 1999:388188 CAPLUS <<LOGINID::20071212>>

DN 131:44836

TI Preparation of novel fused pyridazinones useful as immunosuppressants

IN Bantick, John; Cooper, Martin; Thorne, Philip; Perry, Matthew

PA Astra Pharmaceuticals Ltd., UK; Astra Aktiebolag

SO PCT Int. Appl., 94 pp.

CODEN: PIXXD2

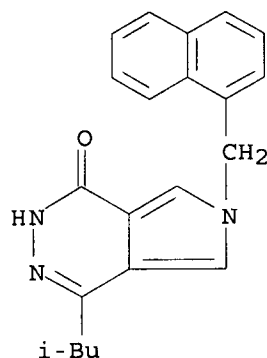
DT Patent

LA English

FAN.CNT 2

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|---|------|----------|-----------------|----------|
| PI | WO 9929695 | A1 | 19990617 | WO 1998-SE2191 | 19981201 |
| | W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW | | | | |
| | RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| | CA 2312419 | A1 | 19990617 | CA 1998-2312419 | 19981201 |
| | AU 9917916 | A | 19990628 | AU 1999-17916 | 19981201 |
| | EP 1036076 | A1 | 20000920 | EP 1998-962754 | 19981201 |
| | EP 1036076 | B1 | 20020904 | | |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO | | | | |
| | BR 9813373 | A | 20001003 | BR 1998-13373 | 19981201 |
| | TR 200001603 | T2 | 20001023 | TR 2000-1603 | 19981201 |
| | EE 200000318 | A | 20010815 | EE 2000-318 | 19981201 |
| | HU 2001000280 | A2 | 20011028 | HU 2001-280 | 19981201 |
| | HU 2001000280 | A3 | 20030328 | | |
| | JP 2001525413 | T | 20011211 | JP 2000-524288 | 19981201 |
| | NZ 504452 | A | 20020531 | NZ 1998-504452 | 19981201 |
| | AT 223413 | T | 20020915 | AT 1998-962754 | 19981201 |
| | US 6342601 | B1 | 20020129 | US 1999-214755 | 19990112 |
| | NO 2000002788 | A | 20000801 | NO 2000-2788 | 20000531 |
| | US 2002099055 | A1 | 20020725 | US 2001-6244 | 20011210 |
| | US 6770646 | B2 | 20040803 | | |
| | US 2004162410 | A1 | 20040819 | US 2004-776245 | 20040212 |
| PRAI | SE 1997-4542 | A | 19971205 | | |
| | SE 1998-1989 | A | 19980604 | | |
| | GB 1995-26273 | A | 19951221 | | |
| | SE 1996-556 | A | 19960215 | | |
| | WO 1996-SE1680 | W | 19961217 | | |
| | US 1997-776231 | A1 | 19970131 | | |
| | WO 1998-SE2191 | W | 19981201 | | |
| | US 1999-214755 | A3 | 19990112 | | |
| | US 1999-353644 | A1 | 19990715 | | |
| | US 2000-708449 | B1 | 20001109 | | |

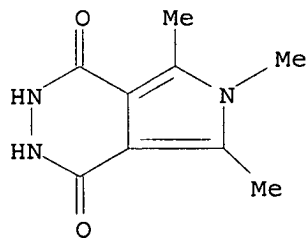
US 2002-74008 B1 20020214
 OS MARPAT 131:44836
 IT 227321-70-2P, 2,6-Dihydro-4-(2-methylpropyl)-6-(1-naphthalenylmethyl)-1H-pyrrolo[3,4-d]pyridazin-1-one
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (intermediate; preparation of fused pyridazinones as immunosuppressants)
 RN 227321-70-2 CAPLUS
 CN 1H-Pyrrolo[3,4-d]pyridazin-1-one, 2,6-dihydro-4-(2-methylpropyl)-6-(1-naphthalenylmethyl)- (CA INDEX NAME)



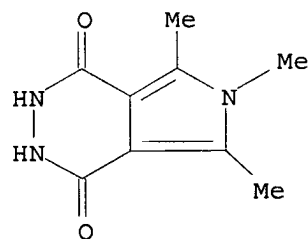
RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 3 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN
 TI Investigation of the structure of and the properties of the potentially tautomeric 1,2,3,4-tetrahydro-5,7-dimethyl-6H-pyrrolo[3,4-d]pyridazine-1,4-diones in the gaseous and aqueous phases using the AM1 semi-empirical method
 AB Potentially tautomeric 1,2,3,4-tetrahydro-5,7-dimethyl-6H-pyrrolo[3,4-d]pyridazine-1,4-diones and their fixed tautomeric forms have been studied in order to predict their tautomeric equilibrium consts. and pKa values using semi-empirical AM1 quantum-chemical calcns. at the SCF level in the gas phase and in aqueous solution Hydroxy-oxo forms were found to be more stable than dioxo and dihydroxy forms. The results obtained from the tautomeric equilibrium and basicity calcns. are in good agreement with exptl. data.
 AN 1998:451319 CAPLUS <<LOGINID::20071212>>
 DN 129:175315
 TI Investigation of the structure of and the properties of the potentially tautomeric 1,2,3,4-tetrahydro-5,7-dimethyl-6H-pyrrolo[3,4-d]pyridazine-1,4-diones in the gaseous and aqueous phases using the AM1 semi-empirical method
 AU Guven, Alaattin; Ogretir, Cemil
 CS Faculty of Science, Chemistry Department, Anadolu University, Eskiehir, Turk.
 SO THEOCHEM (1998), 434, 7-28
 CODEN: THEODJ; ISSN: 0166-1280
 PB Elsevier Science B.V.
 DT Journal
 LA English
 IT 96441-75-7 96441-82-6 211247-93-7
 211247-94-8 211248-10-1 211389-39-8
 211450-67-8
 RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
 (structure of and properties of potentially tautomeric
 1,2,3,4-tetrahydro-5,7-dimethyl-6H-pyrrolo[3,4-d]pyridazine-1,4-diones
 in gaseous and aqueous phases using AM1)

RN 96441-75-7 CAPLUS
 CN 1H-Pyrrolo[3,4-d]pyridazine-1,4(6H)-dione, 2,3-dihydro-5,6,7-trimethyl-
 (CA INDEX NAME)

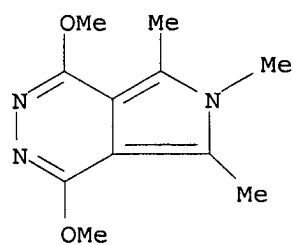


RN 96441-82-6 CAPLUS
 CN 1H-Pyrrolo[3,4-d]pyridazine-1,4(6H)-dione, 2,3-dihydro-5,6,7-trimethyl-,
 conjugate monoacid (9CI) (CA INDEX NAME)

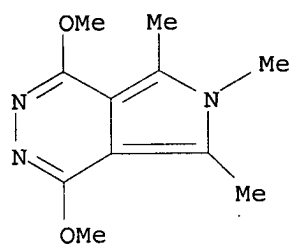


● H⁺

RN 211247-93-7 CAPLUS
 CN 6H-Pyrrolo[3,4-d]pyridazine, 1,4-dimethoxy-5,6,7-trimethyl- (CA INDEX
 NAME)

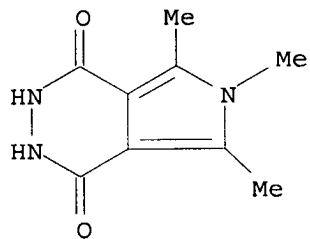


RN 211247-94-8 CAPLUS
 CN 6H-Pyrrolo[3,4-d]pyridazine, 1,4-dimethoxy-5,6,7-trimethyl-, conjugate
 monoacid (9CI) (CA INDEX NAME)



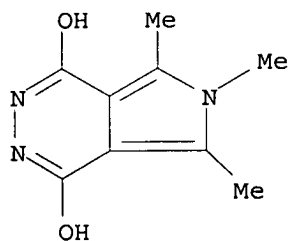
● H⁺

RN 211248-10-1 CAPLUS
 CN 1H-Pyrrolo[3,4-d]pyridazine-1,4(6H)-dione, 2,3-dihydro-5,6,7-trimethyl-, conjugate diacid (9CI) (CA INDEX NAME)

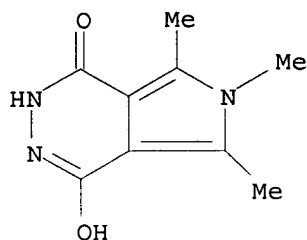


● 2 H⁺

RN 211389-39-8 CAPLUS
 CN 6H-Pyrrolo[3,4-d]pyridazine-1,4-diol, 5,6,7-trimethyl- (CA INDEX NAME)

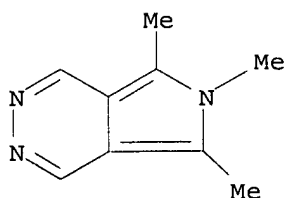


RN 211450-67-8 CAPLUS
 CN 1H-Pyrrolo[3,4-d]pyridazin-1-one, 2,6-dihydro-4-hydroxy-5,6,7-trimethyl- (CA INDEX NAME)

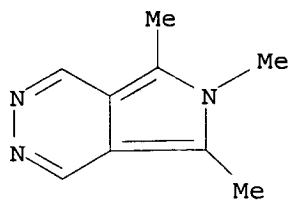


RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 4 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN
 TI Investigation of the structure and properties of the potentially
 tautomeric 5,7-dimethyl-6H-pyrrolo[3,4-d]pyridazines in the gas and
 aqueous phases using the AM1 and PM3/COSMO solvation method
 AB The potentially tautomeric 5,7-dimethyl-6H-pyrrolo[3,4-d]pyridazines, 2H
 and 6H, and their fixed tautomeric forms were studied in order to predict
 the most stable form by the restricted Hartree-Foch approach using
 semiempirical PM3 and AM1 quantum chemical calcns. at the SCF level in the
 gas and aqueous phases. Both methods predicted that the 6H form is more
 stable than the other forms in both gas and aqueous phases. The results
 obtained were found to be in agreement with the exptl. data.
 Monoprotonated forms of 5,7-dimethyl-6H-pyrrolo[3,4-d]pyridazines were
 also examined Proton affinity calcns. predicted that the first protonations
 take place on the N6 atom in the 2H form and on the N2 atom in the 6H
 form, resulting in a common cation.
 AN 1998:220258 CAPLUS <<LOGINID::20071212>>
 DN 128:321258
 TI Investigation of the structure and properties of the potentially
 tautomeric 5,7-dimethyl-6H-pyrrolo[3,4-d]pyridazines in the gas and
 aqueous phases using the AM1 and PM3/COSMO solvation method
 AU Guven, Alaattin; Ogretir, Cemil
 CS Fac. Sci., Chem. Dep., Anadolu Univ., Eskisehir, Turk.
 SO THEOCHEM (1998), 430, 85-95
 CODEN: THEODJ; ISSN: 0166-1280
 PB Elsevier Science B.V.
 DT Journal
 LA English
 IT 30476-58-5 206860-75-5 206860-78-8
 RL: PRP (Properties)
 (AM1 and PM3/COSMO solvation method in study of tautomeric nature of
 5,7-dimethyl-6H-pyrrolo[3,4-d]pyridazines in gas and aqueous phases)
 RN 30476-58-5 CAPLUS
 CN 6H-Pyrrolo[3,4-d]pyridazine, 5,6,7-trimethyl- (8CI, 9CI) (CA INDEX NAME)

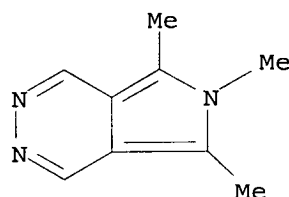


RN 206860-75-5 CAPLUS
 CN 6H-Pyrrolo[3,4-d]pyridazine, 5,6,7-trimethyl-, conjugate monoacid (9CI)
 (CA INDEX NAME)



● H⁺

RN 206860-78-8 CAPLUS
CN 6H-Pyrrolo[3,4-d]pyridazine, 5,6,7-trimethyl-, conjugate diacid (9CI) (CA INDEX NAME)

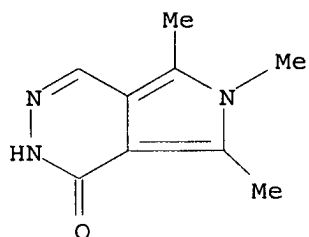


● 2 H⁺

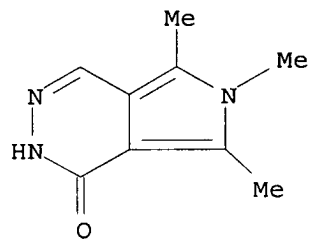
RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 5 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN
TI Investigation of the structure and the properties of the potentially
tautomeric 1,2-dihydro-5,7-dimethyl-6H-pyrrolo[3,4-d]pyridazine-1-ones in
the gas and aqueous phases using semiempirical methods
AB Potentially tautomeric 1,2-dihydro-5,7-dimethyl-6H-pyrrolo[3,4-
d]pyridazine-1-ones and their fixed tautomeric forms have been studied, in
order to predict their tautomeric equilibrium consts. and pKa values, using
semiempirical PM3, AM1 quantum-chemical calcns. at the SCF level in the gas
phase and in aqueous solution The effect of alkylation on the pKa value was
also investigated. In both the gas phase and in aqueous solution, oxo forms have
been found to be more stable than hydroxy and zwitterionic structures. The
results obtained from the tautomeric equilibrium and acidity calcns. are in
good agreement with exptl. data.
AN 1998:199391 CAPLUS <<LOGINID::20071212>>
DN 129:4401
TI Investigation of the structure and the properties of the potentially
tautomeric 1,2-dihydro-5,7-dimethyl-6H-pyrrolo[3,4-d]pyridazine-1-ones in
the gas and aqueous phases using semiempirical methods
AU Guven, Alaatin; Ogretir, Cemil
CS Fac. Sci., Chem. Dep., Anadolu Univ., Eskisehir, Turk.
SO THEOCHEM (1998), 427, 65-77
CODEN: THEODJ; ISSN: 0166-1280
PB Elsevier Science B.V.

DT Journal
 LA English
 IT 90817-87-1 96441-64-4 207286-20-2
 207286-21-3 207286-22-4 207286-23-5
 207286-24-6 207286-25-7 207286-26-8
 207355-02-0 207355-03-1 207355-04-2
 RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT
 (Reactant); PROC (Process); RACT (Reactant or reagent)
 (structure and properties of potentially tautomeric
 1,2-dihydro-5,7-dimethyl-6H-pyrrolo[3,4-d]pyridazine-1-ones in gas and
 aqueous phases using semiempirical methods)
 RN 90817-87-1 CAPLUS
 CN 1H-Pyrrolo[3,4-d]pyridazin-1-one, 2,6-dihydro-5,6,7-trimethyl- (CA INDEX
 NAME)

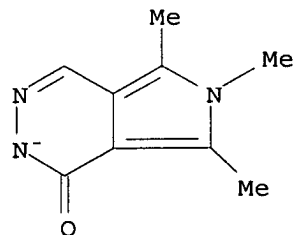


RN 96441-64-4 CAPLUS
 CN 1H-Pyrrolo[3,4-d]pyridazin-1-one, 2,6-dihydro-5,6,7-trimethyl-, conjugate
 monoacid (9CI) (CA INDEX NAME)

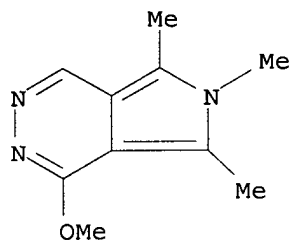


● H⁺

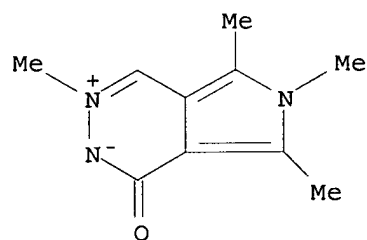
RN 207286-20-2 CAPLUS
 CN 1H-Pyrrolo[3,4-d]pyridazin-1-one, 2,6-dihydro-5,6,7-trimethyl-, ion(1-)
 (CA INDEX NAME)



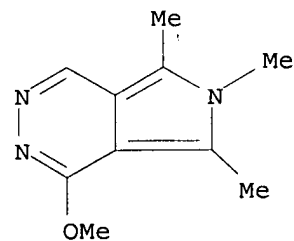
RN 207286-21-3 CAPLUS
 CN 6H-Pyrrolo[3,4-d]pyridazine, 1-methoxy-5,6,7-trimethyl- (CA INDEX NAME)



RN 207286-22-4 CAPLUS
 CN 1H-Pyrrolo[3,4-d]pyridazinium, 2,6-dihydro-3,5,6,7-tetramethyl-1-oxo-,
 inner salt (CA INDEX NAME)

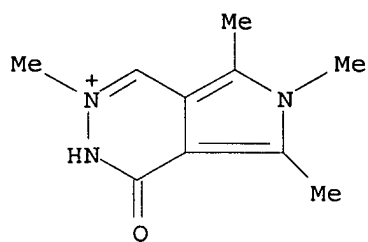


RN 207286-23-5 CAPLUS
 CN 6H-Pyrrolo[3,4-d]pyridazine, 1-methoxy-5,6,7-trimethyl-, conjugate
 monoacid (9CI) (CA INDEX NAME)



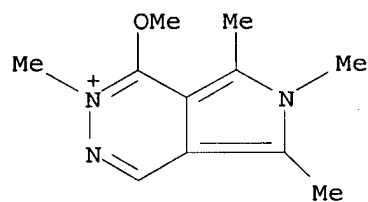
● H⁺

RN 207286-24-6 CAPLUS
 CN 1H-Pyrrolo[3,4-d]pyridazinium, 2,6-dihydro-3,5,6,7-tetramethyl-1-oxo- (CA
 INDEX NAME)



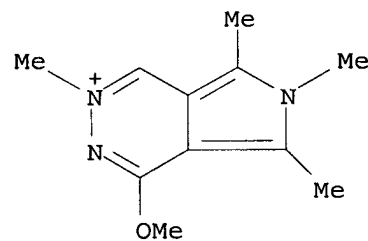
RN 207286-25-7 CAPLUS

CN 6H-Pyrrolo[3,4-d]pyridazinium, 1-methoxy-2,5,6,7-tetramethyl- (CA INDEX NAME)



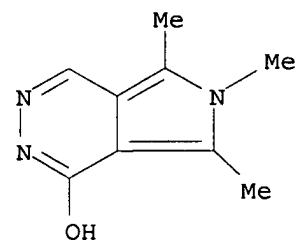
RN 207286-26-8 CAPLUS

CN 6H-Pyrrolo[3,4-d]pyridazinium, 4-methoxy-2,5,6,7-tetramethyl- (CA INDEX NAME)



RN 207355-02-0 CAPLUS

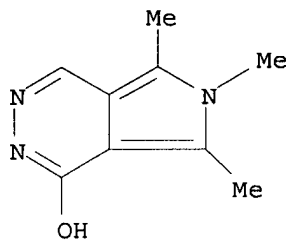
CN 6H-Pyrrolo[3,4-d]pyridazin-1-ol, 5,6,7-trimethyl-, conjugate monoacid (9CI) (CA INDEX NAME)



● H⁺

RN 207355-03-1 CAPLUS

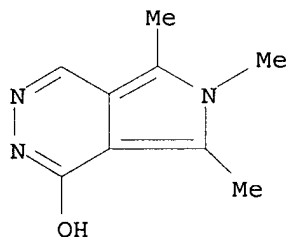
CN 6H-Pyrrolo[3,4-d]pyridazin-1-ol, 5,6,7-trimethyl-, conjugate diacid (9CI)
(CA INDEX NAME)



● 2 H⁺

RN 207355-04-2 CAPLUS

CN 6H-Pyrrolo[3,4-d]pyridazin-1-ol, 5,6,7-trimethyl- (CA INDEX NAME)

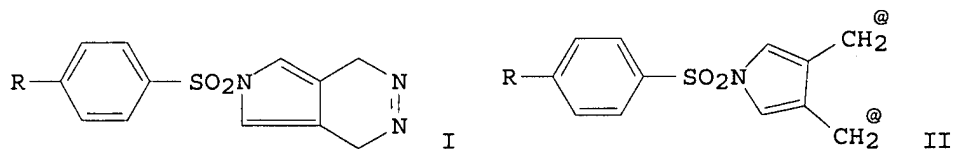


RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 6 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN

TI Long-lived spin isomerism of singlet and triplet states of
N-arenesulfonyl-3,4-dimethylenepyrroles

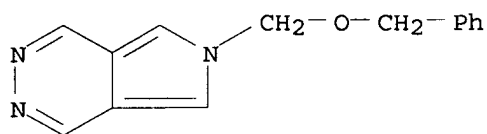
GI



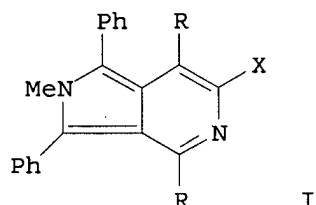
AB A theor. prediction that attachment of an electron-withdrawing group to the ring nitrogen of a 3,4-dimethylenepyrrole biradical should selectively stabilize the triplet state is tested by generation of matrix-immobilized transient species in the irradiation of 1,4-dihydro-6-arenesulfonylpyrrolo[3,4-d]pyridazine precursors (I; R = Me, Br) at 265 nm. ESR spectra of triplet species assigned to the corresponding dimethylenepyrroles (II) are observed in both cases. The zero-field splitting parameter D is 0.023 cm⁻¹ in both cases, essentially the same as those reported in the literature for

tetramethyleneethane derivs. Irradiation of the precursors at 370 nm gives rise in both cases to the corresponding singlets, blue (λ_{max} 593 and 600 nm, resp.), ESR-silent substances. The spin isomers do not interconvert over a period of days.

AN 1994:133629 CAPLUS <<LOGINID::20071212>>
 DN 120:133629
 TI Long-lived spin isomerism of singlet and triplet states of
 N-arenesulfonyl-3,4-dimethylenepyrroles
 AU Bush, Linda C.; Heath, Richard B.; Berson, Jerome A.
 CS Dep. Chem., Yale Univ., New Haven, CT, 06511, USA
 SO Journal of the American Chemical Society (1993), 115(21), 9830-1
 CODEN: JACSAT; ISSN: 0002-7863
 DT Journal
 LA English
 IT 152940-60-8P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and reduction of)
 RN 152940-60-8 CAPLUS
 CN 6H-Pyrrolo[3,4-d]pyridazine, 6-[(phenylmethoxy)methyl]- (CA INDEX NAME)

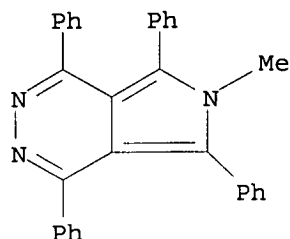


L9 ANSWER 7 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN
 TI Substituent effects on the spectra of fluorescent aryl-substituted
 N-methylpyrrolo[3,4-c]pyridines
 GI

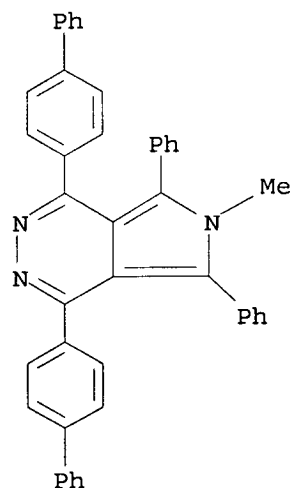


AB Introduction of an alkoxy group into the Ph ring at the 4 and 7 positions of I (R = aryl; X = CN, CONH2, CO2H) had little effect on the absorption and emission spectra of the title dyes, while introduction of a Br group caused a red shift in the spectrum of I (X = CN). I (X = CN, CO2Et, H) were strongly fluorescent, while the fluorescence of I (X = CONH2) was weak; I (X = CONHNH2, CO2H) were also weakly fluorescent with a large Stokes shift (.apprx.150 nm). Related pyridazines were not fluorescent.
 AN 1993:82819 CAPLUS <<LOGINID::20071212>>
 DN 118:82819
 TI Substituent effects on the spectra of fluorescent aryl-substituted
 N-methylpyrrolo[3,4-c]pyridines
 AU Mataka, Shuntaro; Tashiro, Masashi; Misumi, Osamu; Lin, Wei Hua;
 Takahashi, Kazufumi; Torii, Akiyoshi
 CS Inst. Adv. Mater. Study, Kyushu Univ., Kasuga, 816, Japan
 SO Dyes and Pigments (1992), 20(2), 83-96
 CODEN: DYPIDX; ISSN: 0143-7208

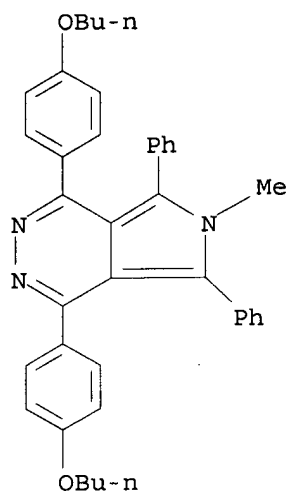
DT Journal
 LA English
 IT 145551-53-7P 145551-54-8P 145551-55-9P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (preparation and fluorescence of, substituent effect in relation to)
 RN 145551-53-7 CAPLUS
 CN 6H-Pyrrolo[3,4-d]pyridazine, 6-methyl-1,4,5,7-tetraphenyl- (CA INDEX NAME)



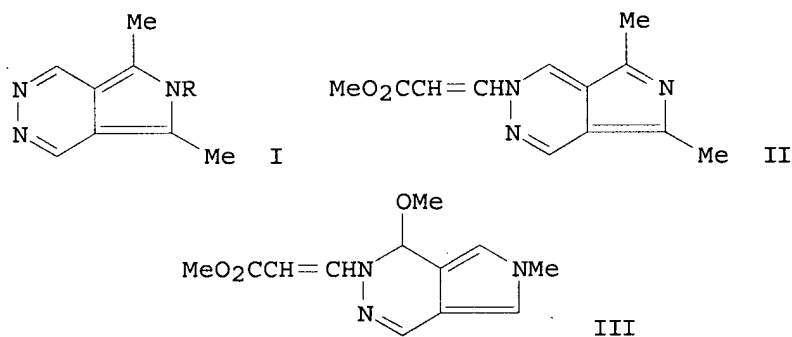
RN 145551-54-8 CAPLUS
 CN 6H-Pyrrolo[3,4-d]pyridazine, 1,4-bis([1,1'-biphenyl]-4-yl)-6-methyl-5,7-diphenyl- (CA INDEX NAME)



RN 145551-55-9 CAPLUS
 CN 6H-Pyrrolo[3,4-d]pyridazine, 1,4-bis(4-butoxyphenyl)-6-methyl-5,7-diphenyl- (CA INDEX NAME)

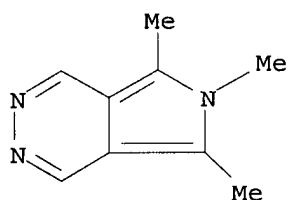


L9 ANSWER 8 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN
 TI Pyrrole studies. Part 39. The disparate reactivity of
 5,7-dimethyl-6H-pyrrolo[3,4-d]pyridazines with acetylenic esters and with
 azodicarboxylic esters
 GI

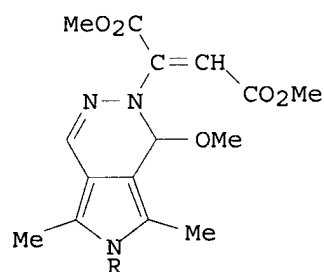
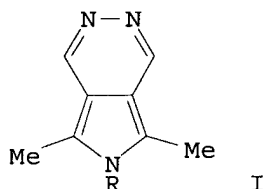


AB Reaction of MeO2CC.tplbond.CH with the title pyrrolopyridazines I (R = H,
 Me) in MeOH gave adducts II and III, resp., but no ring opened products.
 In contrast, EtO2CN:NCO2Et underwent reaction with I (R = H) at the
 electron-rich 5-membered ring.
 AN 1988:510358 CAPLUS <<LOGINID::20071212>>
 DN 109:110358
 TI Pyrrole studies. Part 39. The disparate reactivity of
 5,7-dimethyl-6H-pyrrolo[3,4-d]pyridazines with acetylenic esters and with
 azodicarboxylic esters
 AU Fuentes Rodriguez, Fernanda; Sepulveda-Arques, Jose; Jones, R. Alan
 CS Fac. Farm., Univ. Valencia, Valencia, 46010, Spain
 SO Journal of Chemical Research, Synopses (1987), (11), 356
 CODEN: JRPSDC; ISSN: 0308-2342
 DT Journal
 LA English
 OS CASREACT 109:110358
 IT 30476-58-5
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (addition reaction of, with Me propiolate)
 RN 30476-58-5 CAPLUS

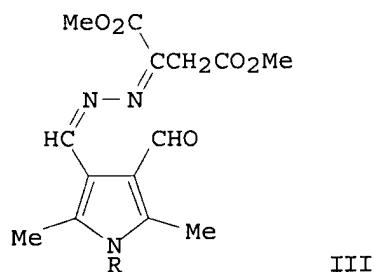
CN 6H-Pyrrolo[3,4-d]pyridazine, 5,6,7-trimethyl- (8CI, 9CI) (CA INDEX NAME)



L9 ANSWER 9 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN
TI Pyrrole studies. Part 32. A novel ring-cleavage reaction of the
pyridazine ring during the reaction of 6H-pyrrolo[3,4-d]pyridazines with
dimethyl acetylenedicarboxylate
GI



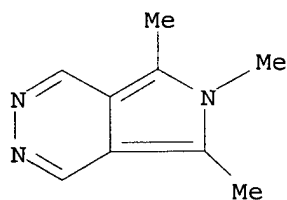
II



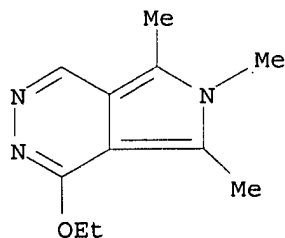
III

AB Treatment of pyrrolopyridazines I (R = Me, H, Ph) with (MeO2CC.tplbond.)₂
in MeOH at -70° gave the corresponding esters II (R as before),
which were unstable in the presence of H₂O and underwent ring cleavage to
the corresponding pyrroles III. The structure of III (R = H) was
confirmed by x-ray anal.
AN 1985:471267 CAPLUS <<LOGINID::20071212>>
DN 103:71267
TI Pyrrole studies. Part 32. A novel ring-cleavage reaction of the
pyridazine ring during the reaction of 6H-pyrrolo[3,4-d]pyridazines with
dimethyl acetylenedicarboxylate
AU Hernandez de la Figuera Gomez, Teresa; Sepulveda Arques, Jose; Jones, R.
Alan; Dawes, Helen M.; Hursthouse, Michael B.
CS Dep. Quim. Org., Univ. Valencia, Valencia, Spain
SO Journal of the Chemical Society, Perkin Transactions 1: Organic and
Bio-Organic Chemistry (1972-1999) (1985), (4), 899-902
CODEN: JCPRB4; ISSN: 0300-922X
DT Journal
LA English
OS CASREACT 103:71267

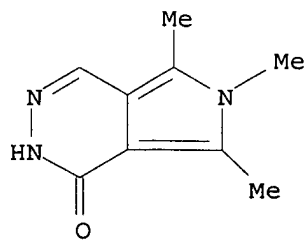
IT 30476-58-5
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with di-Me acetylenedicarboxylate)
 RN 30476-58-5 CAPLUS
 CN 6H-Pyrrolo[3,4-d]pyridazine, 5,6,7-trimethyl- (8CI, 9CI) (CA INDEX NAME)



L9 ANSWER 10 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN
 TI Pyrrole studies: 31. The structures of potentially tautomeric
 1,2-dihydro-6H-pyrrolo[3,4-d]pyridazin-1-ones and 1,2,3,4-tetrahydro-6H-
 pyrrolo[3,4-d]pyridazine-1,4-diones
 AB 1,2-Dihydro-6H-pyrrolo[3,4-d]pyridazin-1-ones exist predominantly as such
 in equilibrium with the 1-hydroxypyridazine form, whereas
 1,2,3,4-tetrahydro-6H-
 pyrrolo[3,4-d]pyridazine-1,4-diones in equilibrium with the monohydroxy-oxo
 tautomeric forms are preferred by a factor of only .apprx.100:1. It was
 not possible to determine the position of equilibrium between the
 1-hydroxy-6H-pyrrolo[3,4-d]pyridazin-4-one and the 1,4-dihydroxy-6H-
 pyrrolo[3,4-d]pyridazine structures.
 AN 1985:422083 CAPLUS <<LOGINID::20071212>>
 DN 103:22083
 TI Pyrrole studies: 31. The structures of potentially tautomeric
 1,2-dihydro-6H-pyrrolo[3,4-d]pyridazin-1-ones and 1,2,3,4-tetrahydro-6H-
 pyrrolo[3,4-d]pyridazine-1,4-diones
 AU Inel, Sermin; Jones, R. Alan; Ogretir, Cemil
 CS Sch. Chem. Sci., Univ. East Anglia, Norwich, NR4 7TJ, UK
 SO Tetrahedron (1984), 40(20), 3979-86
 CODEN: TETRAB; ISSN: 0040-4020
 DT Journal
 LA English
 OS CASREACT 103:22083
 IT 96441-62-2 96441-64-4 96441-67-7
 96441-69-9 96441-72-4 96441-73-5
 96441-80-4 96441-82-6 96441-86-0
 96441-88-2
 RL: PRP (Properties)
 (UV spectrum of)
 RN 96441-62-2 CAPLUS
 CN 6H-Pyrrolo[3,4-d]pyridazine, 1-ethoxy-5,6,7-trimethyl- (CA INDEX NAME)

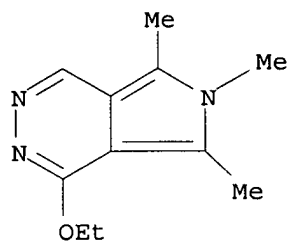


RN 96441-64-4 CAPLUS
CN 1H-Pyrrolo[3,4-d]pyridazin-1-one, 2,6-dihydro-5,6,7-trimethyl-, conjugate
monoacid (9CI) (CA INDEX NAME)



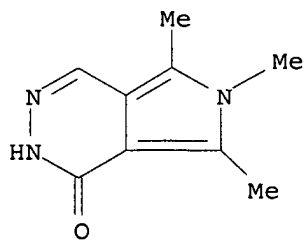
● H⁺

RN 96441-67-7 CAPLUS
CN 6H-Pyrrolo[3,4-d]pyridazine, 1-ethoxy-5,6,7-trimethyl-, conjugate monoacid
(9CI) (CA INDEX NAME)



● H⁺

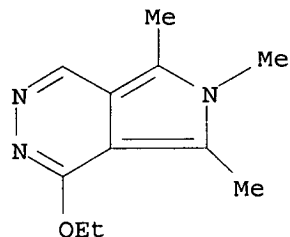
RN 96441-69-9 CAPLUS
CN 1H-Pyrrolo[3,4-d]pyridazin-1-one, 2,6-dihydro-5,6,7-trimethyl-, conjugate
diacid (9CI) (CA INDEX NAME)



● 2 H⁺

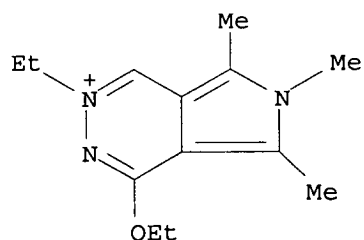
RN 96441-72-4 CAPLUS

CN 6H-Pyrrolo[3,4-d]pyridazine, 1-ethoxy-5,6,7-trimethyl-, conjugate diacid
(9CI) (CA INDEX NAME)



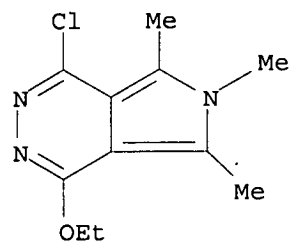
● 2 H⁺

RN 96441-73-5 CAPLUS
CN 6H-Pyrrolo[3,4-d]pyridazinium, 4-ethoxy-2-ethyl-5,6,7-trimethyl-,
conjugate monoacid (9CI) (CA INDEX NAME)

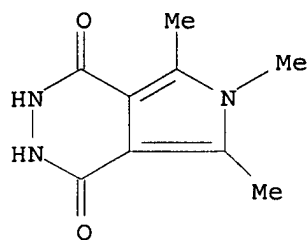


● H⁺

RN 96441-80-4 CAPLUS
CN 6H-Pyrrolo[3,4-d]pyridazine, 1-chloro-4-ethoxy-5,6,7-trimethyl- (CA INDEX
NAME)

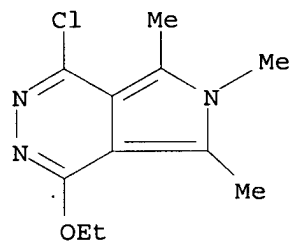


RN 96441-82-6 CAPLUS
CN 1H-Pyrrolo[3,4-d]pyridazine-1,4(6H)-dione, 2,3-dihydro-5,6,7-trimethyl-,
conjugate monoacid (9CI) (CA INDEX NAME)



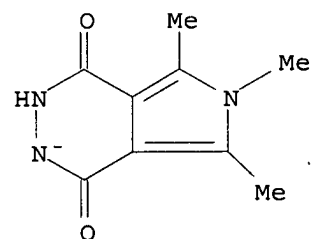
● H⁺

RN 96441-86-0 CAPLUS
 CN 6H-Pyrrolo[3,4-d]pyridazine, 1-chloro-4-ethoxy-5,6,7-trimethyl-, conjugate monoacid (9CI) (CA INDEX NAME)

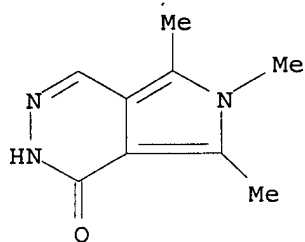


● H⁺

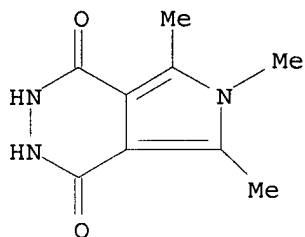
RN 96441-88-2 CAPLUS
 CN 1H-Pyrrolo[3,4-d]pyridazine-1,4(6H)-dione, 2,3-dihydro-5,6,7-trimethyl-, ion(1-) (CA INDEX NAME)



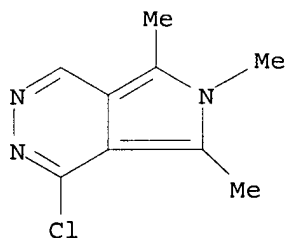
IT 90817-87-1 96441-75-7
 RL: PRP (Properties)
 (UV spectrum of, absence of tautomerism in relation to)
 RN 90817-87-1 CAPLUS
 CN 1H-Pyrrolo[3,4-d]pyridazin-1-one, 2,6-dihydro-5,6,7-trimethyl- (CA INDEX NAME)



RN 96441-75-7 CAPLUS
 CN 1H-Pyrrolo[3,4-d]pyridazine-1,4(6H)-dione, 2,3-dihydro-5,6,7-trimethyl-
 (CA INDEX NAME)

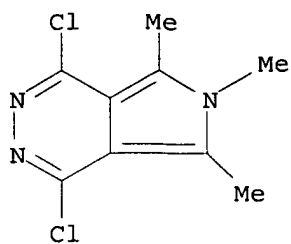


IT 96441-91-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and reaction with sodium methoxide)
 RN 96441-91-7 CAPLUS
 CN 6H-Pyrrolo[3,4-d]pyridazine, 1-chloro-5,6,7-trimethyl-, monohydrochloride
 (9CI) (CA INDEX NAME)



● HCl

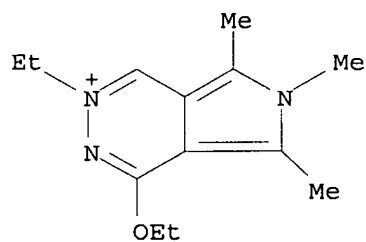
IT 96441-92-8P 96452-45-8P 96452-47-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 96441-92-8 CAPLUS
 CN 6H-Pyrrolo[3,4-d]pyridazine, 1,4-dichloro-5,6,7-trimethyl- (CA INDEX
 NAME)



RN 96452-45-8 CAPLUS
 CN 6H-Pyrrolo[3,4-d]pyridazinium, 4-ethoxy-2-ethyl-5,6,7-trimethyl-,
 tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

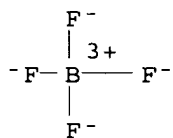
CM 1

CRN 96452-44-7
 CMF C13 H20 N3 O



CM 2

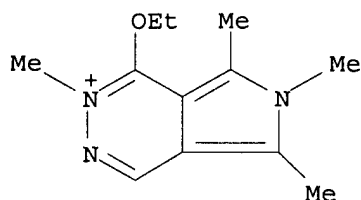
CRN 14874-70-5
 CMF B F4
 CCI CCS



RN 96452-47-0 CAPLUS
 CN 6H-Pyrrolo[3,4-d]pyridazinium, 1-ethoxy-2,5,6,7-tetramethyl-,
 tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 96452-46-9
 CMF C12 H18 N3 O

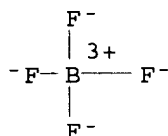


CM 2

CRN 14874-70-5

CMF B F4

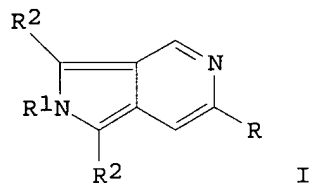
CCI CCS



L9 ANSWER 11 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN

TI Structure and reactivity of iso-fused heterocyclic systems with $4n \pi$ and $(4n + 2) \pi$ electrons. 8. Cyclizing condensation of 1H-pyrrole-3,4-dicarbaldehydes with 1,2-bifunctional compounds. A general and simple preparation method for 2H-pyrrolo[3,4-c]pyridines and 6H-pyrrolo[3,4-d]pyridazines

GI



AB 2H-Pyrrolo[3,4-c]pyridines I ($R = \text{CO}_2\text{Me}, \text{CO}_2\text{Et}, \text{cyano}$; $R_1 = \text{H}, \text{Me}, \text{CMe}_3, \text{CH}_2\text{Ph}$; $R_2 = \text{H}, \text{Me}$) are easily and efficiently accessible via reaction of 1H-pyrrole-3,4-dicarbaldehydes with $\text{H}_2\text{NCH}_2\text{R} \cdot \text{HCl}$. Under the influence of Et_2NH the cyclocondensation occurs in an uniform fashion and in 55-99% yields. In a similar manner 1H-pyrrole-3,4-dicarbaldehydes react with N_2H_4 ; two-fold elimination of H_2O leads to 6H-pyrrolo[3,4-d]pyridazines. The bicyclic hetarenes are stabilized compared with 2H-isoindoles by addnl. heteroatoms in the 6-membered ring and acceptor groups at the 6-position.

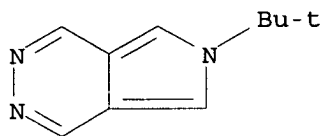
AN 1985:45802 CAPLUS <<LOGINID::20071212>>

DN 102:45802

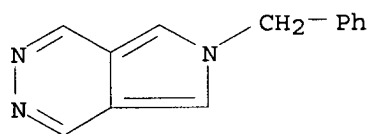
TI Structure and reactivity of iso-fused heterocyclic systems with $4n \pi$ and $(4n + 2) \pi$ electrons. 8. Cyclizing condensation of 1H-pyrrole-3,4-dicarbaldehydes with 1,2-bifunctional compounds. A general and simple preparation method for 2H-pyrrolo[3,4-c]pyridines and 6H-pyrrolo[3,4-d]pyridazines

AU Kreher, Richard P.; Pfister, Juergen

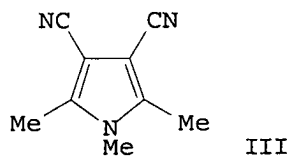
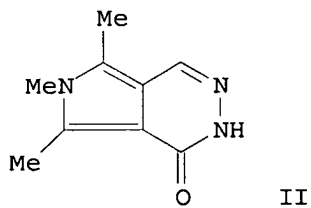
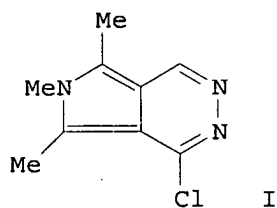
CS Abt. Chem., Univ. Dortmund, Dortmund, D-4600/50, Fed. Rep. Ger.
 SO Chemiker-Zeitung (1984), 108(9), 275-7
 CODEN: CMKZAT; ISSN: 0009-2894
 DT Journal
 LA German
 OS CASREACT 102:45802
 IT 94169-85-4P 94169-86-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 94169-85-4 CAPLUS
 CN 6H-Pyrrolo[3,4-d]pyridazine, 6-(1,1-dimethylethyl)- (CA INDEX NAME)



RN 94169-86-5 CAPLUS
 CN 6H-Pyrrolo[3,4-d]pyridazine, 6-(phenylmethyl)- (CA INDEX NAME)



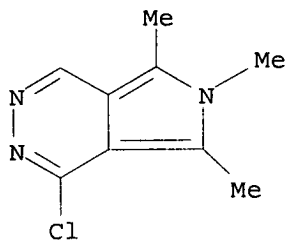
L9 ANSWER 12 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN
 TI Pyrrole studies. XXIX. An unusual pyridazine ring-opening reaction
 GI



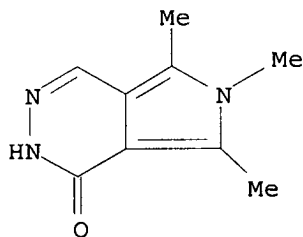
AB Treating 1-chloro-5,6,7-trimethylpyrrolo[3,4-d]pyridazine (I) with aqueous or alc. NaOH, NaOEt, or NaOPh gave approx. 60% pyridazinone II. Treating I with NaOMe in DMF gave 42% dicyanopyrrole III and 40% II; NaOEt in DMF gave 19% III.

AN 1984:423418 CAPLUS <<LOGINID::20071212>>
 DN 101:23418
 TI Pyrrole studies. XXIX. An unusual pyridazine ring-opening reaction
 AU Jones, R. Alan; Inel, Sermin
 CS Sch. Chem. Sci., Univ. East Anglia, Norwich, NR4 7TJ, UK
 SO Chemistry & Industry (London, United Kingdom) (1984), (7), 270-1
 CODEN: CHINAG; ISSN: 0009-3068
 DT Journal
 LA English
 OS CASREACT 101:23418

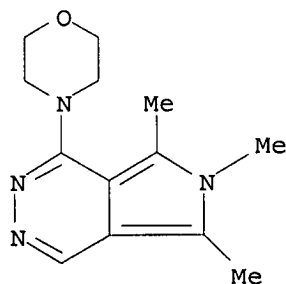
IT 90817-88-2
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (base-catalyzed ring cleavage of)
 RN 90817-88-2 CAPLUS
 CN 6H-Pyrrolo[3,4-d]pyridazine, 1-chloro-5,6,7-trimethyl- (CA INDEX NAME)



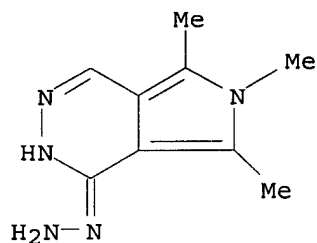
IT 90817-87-1P
 RL: FORM (Formation, nonpreparative); PREP (Preparation)
 (formation of, in ring cleavage of chlorotrimethylpyrrolopyridazine)
 RN 90817-87-1 CAPLUS
 CN 1H-Pyrrolo[3,4-d]pyridazin-1-one, 2,6-dihydro-5,6,7-trimethyl- (CA INDEX NAME)



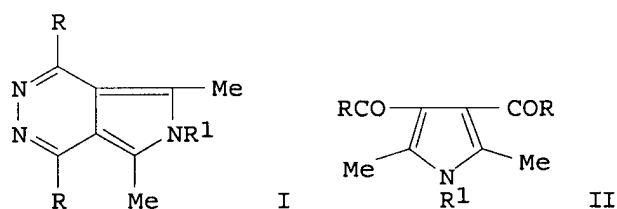
IT 90817-90-6P 90817-91-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 90817-90-6 CAPLUS
 CN 6H-Pyrrolo[3,4-d]pyridazine, 5,6,7-trimethyl-1-(4-morpholinyl)- (CA INDEX NAME)



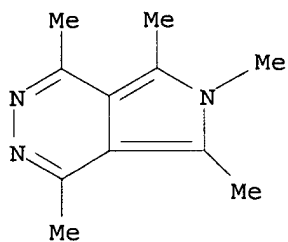
RN 90817-91-7 CAPLUS
 CN 1H-Pyrrolo[3,4-d]pyridazin-1-one, 2,6-dihydro-5,6,7-trimethyl-, hydrazone
 (9CI) (CA INDEX NAME)



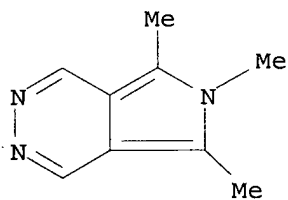
L9 ANSWER 13 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN
 TI Pyrrole studies. XXV. Structure of potentially tautomeric
 pyrrolo[3,4-d]pyridazines
 GI



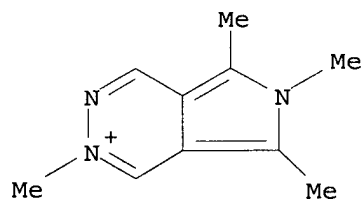
AB Pyrrolopyridazines I (R = H, Me, R1 = H) were prepared by treating the
 pyrroles II with N2H4. II (R = R1 = H) was obtained by formylating
 2,5-dimethylpyrrole and II (R = Me, R1 = H) from Ac2CHCHAc2 and NH4OAc.
 Methylation gave II (R = H, Me, R1 = Me) which were treated with N2H4 to
 give I (R = H, Me, R1 = Me). Quaternized derivs. were obtained with
 MeNHNH2 and MeNHNHMe or by quaternizing I. Electron spectra and basicity
 measurement showed that I exist in a 6H-form in accordance with MO calcns.
 of the relative resonance energies of the possible tautomers. Protonation
 occurs at the heteroatoms and at C-5.
 AN 1981:569111 CAPLUS <<LOGINID::20071212>>
 DN 95:169111
 OREF 95:28269a,28272a
 TI Pyrrole studies. XXV. Structure of potentially tautomeric
 pyrrolo[3,4-d]pyridazines
 AU Acar, Fatma; Badesha, Santokh Singh; Flitsch, Wilhelm; Gozogul, Reyhan;
 Inel, Oguz; Inel, Sermin; Jones, R. Alan; Ogretir, Cemil; Rustidge, David
 C.
 CS Kim. Lab., Devlet Mimarlik Muhendislik Akad., Eskisehir, Turk.
 SO Chimica Acta Turcica (1981), 9(1), 225-37
 CODEN: CATUA9; ISSN: 0379-5896
 DT Journal
 LA English
 OS CASREACT 95:169111
 IT 79398-46-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and quaternization of)
 RN 79398-46-2 CAPLUS
 CN 6H-Pyrrolo[3,4-d]pyridazine, 1,4,5,6,7-pentamethyl- (CA INDEX NAME)



IT 30476-58-5P 79398-41-7P 79398-43-9P
 79398-49-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 30476-58-5 CAPLUS
 CN 6H-Pyrrolo[3,4-d]pyridazine, 5,6,7-trimethyl- (8CI, 9CI) (CA INDEX NAME)



RN 79398-41-7 CAPLUS
 CN 6H-Pyrrolo[3,4-d]pyridazinium, 2,5,6,7-tetramethyl-, iodide (9CI) (CA INDEX NAME)

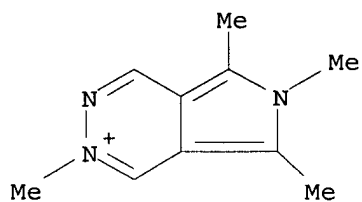


● I⁻

RN 79398-43-9 CAPLUS
 CN 6H-Pyrrolo[3,4-d]pyridazinium, 2,5,6,7-tetramethyl-, sulfate (1:1) (CA INDEX NAME)

CM 1

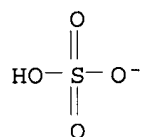
CRN 79398-42-8
 CMF C10 H14 N3



CM 2

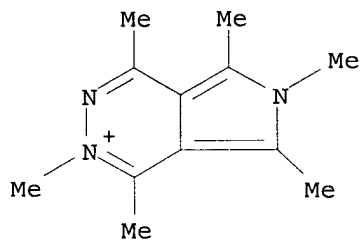
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CMF H O4 S



RN 79398-49-5 CAPLUS

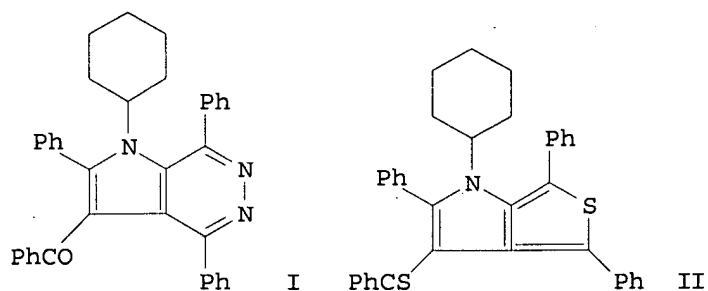
CN 6H-Pyrrolo[3,4-d]pyridazinium, 1,2,4,5,6,7-hexamethyl-, iodide (9CI) (CA INDEX NAME)



L9 ANSWER 14 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN

TI Synthetic approaches to fused heteroaromatic compounds by the condensation reactions of functional pyrroles

GI



AB Diacyl- and triacylpyrroles, obtained by one pot synthesis from aziridines and acetylenic dipolarophiles, underwent condensation reactions. On treatment of 3,4-di- and 2,3,4-tribenzoylpyrroles with hydrazine hydrate and phosphorus pentasulfide, pyrrolopyridazine derivs., e.g. I, and fused thiophenes, e.g. II, resp., were prepared. The structure proofs for I were based on the ^{13}C FT-NMR spectrum of the corresponding ^{13}C -enriched compds.

AN 1978:443293 CAPLUS <<LOGINID::20071212>>

DN 89:43293

OREF 89:6725a,6728a

TI Synthetic approaches to fused heteroaromatic compounds by the condensation reactions of functional pyrroles

AU Uchida, Takane

CS Fac. Educ., Fukui Univ., Fukui, Japan

SO Journal of Heterocyclic Chemistry (1978), 15(2), 241-8

CODEN: JHTCAD; ISSN: 0022-152X

DT Journal

LA English

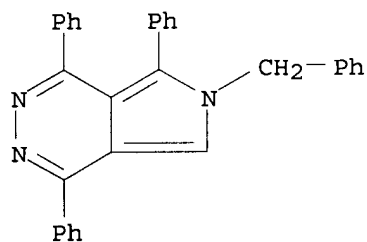
OS CASREACT 89:43293

IT 66864-43-5P 66864-44-6P 66939-89-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

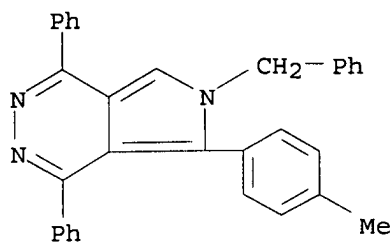
RN 66864-43-5 CAPLUS

CN 6H-Pyrrolo[3,4-d]pyridazine, 1,4,5-triphenyl-6-(phenylmethyl)- (CA INDEX NAME)

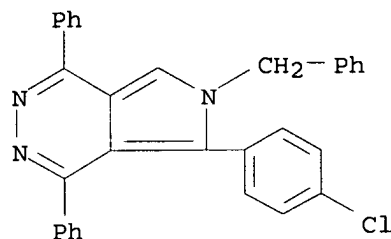


RN 66864-44-6 CAPLUS

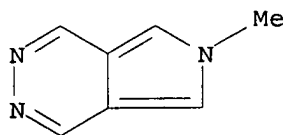
CN 6H-Pyrrolo[3,4-d]pyridazine, 5-(4-methylphenyl)-1,4-diphenyl-6-(phenylmethyl)- (CA INDEX NAME)



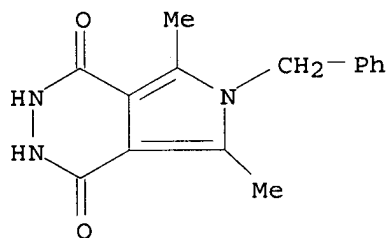
RN 66939-89-7 CAPLUS
 CN 6H-Pyrrolo[3,4-d]pyridazine, 5-(4-chlorophenyl)-1,4-dimethyl-6-(phenylmethyl)- (9CI) (CA INDEX NAME)



L9 ANSWER 15 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN
 TI Synthesis of new condensed pyrrolic heterocycles
 GI For diagram(s), see printed CA Issue.
 AB 1-Methyl-3,4-diformylpyrrole (I, R = CHO) (prepared by reduction of I (R = CO₂Et) to give I (R = CH₂OH) followed by oxidation with Ag₂CO₃) condensed with (MeO₂CCH₂)₂CO, Et₂CO, N₂H₄, and with H₂NCH₂CO₂Et to give the condensed heterocycles II (R = CO₂Me and Me) and III (X = N and CCO₂Et), resp.
 AN 1974:3411 CAPLUS <<LOGINID::20071212>>
 DN 80:3411
 OREF 80:595a,598a
 TI Synthesis of new condensed pyrrolic heterocycles
 AU Duflos, J.; Letouze, D.; Queguiner, G.; Pastour, P.
 CS Inst. Nat. Super. Chim. Ind., Rouen, Fr.
 SO Tetrahedron Letters (1973), (36), 3453-4
 CODEN: TELEAY; ISSN: 0040-4039
 DT Journal
 LA French
 IT 51110-68-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 51110-68-0 CAPLUS
 CN 2H-Pyrrolo[3,4-d]pyridazine, 2-methyl- (9CI) (CA INDEX NAME)

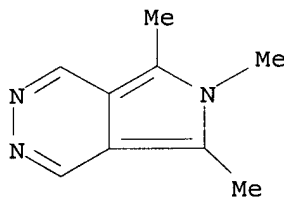


L9 ANSWER 16 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN
 TI Syntheses of pyridazino[1,2-a]pyridazine derivatives of furan, pyridazine, and pyrrole by Diels-Alder reactions
 GI For diagram(s), see printed CA Issue.
 AB Diels-Alder adducts were formed in the Pb(OAc)₄ oxidations of substituted cyclic hydrazides of furan, pyridazine, and pyrrole dicarboxylic acids in the presence of 1,3-cyclohexadiene or 1,3-cyclopentadiene. The products resulting were furo[3,4-g]pyridazino[1,2-a]pyridazine-6,10-diones (I), pyridazino[4,5-g]pyridazino[1,2-a]pyridazine-6,11-diones (II), and pyrrolo[3,4-g]pyridazino[1,2-a]pyridazine-6,10-diones (III), resp. Some hydrogenations and ring opening reactions were studied.
 AN 1971:99966 CAPLUS <<LOGINID::20071212>>
 DN 74:99966
 OREF 74:16277a,16280a
 TI Syntheses of pyridazino[1,2-a]pyridazine derivatives of furan, pyridazine, and pyrrole by Diels-Alder reactions
 AU Gillis, Bernard T.; Valentour, James C.
 CS Dep. Chem., Duquesne Univ., Pittsburgh, PA, USA
 SO Journal of Heterocyclic Chemistry (1971), 8(1), 13-17
 CODEN: JHTCAD; ISSN: 0022-152X
 DT Journal
 LA English
 IT 31379-83-6P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 31379-83-6 CAPLUS
 CN 1H-Pyrrolo[3,4-d]pyridazine-1,4(6H)-dione, 6-benzyl-2,3-dihydro-5,7-dimethyl- (8CI) (CA INDEX NAME)



L9 ANSWER 17 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN
 TI Structure and reactivity of isocondensed heterocyclic systems with 4n and (4m+2) π -electrons. 2. Cyclizing condensation of 3,4-pyrroledicarboxaldehydes with compounds containing acidic CH and NH groups
 GI For diagram(s), see printed CA Issue.
 AB 6-Carbethoxy-1,2,3-trimethyl-2H-pyrrolo[3,4-c]-pyridine (I) is prepared by the reaction of 1,2,5-trimethyl-3,4-pyrroledicarboxaldehyde (II) with H₂NCH₂CO₂Et; 1,2,3-trimethyl-2H-pyrrolo[3,4-d]pyridazine (III) is prepared from N₂H₄. II is treated with RCH₂CH₂R (R = Bz, CN) to give the corresponding 2H-isoindoles (IV).
 AN 1971:53695 CAPLUS <<LOGINID::20071212>>
 DN 74:53695
 OREF 74:8657a
 TI Structure and reactivity of isocondensed heterocyclic systems with 4n and (4m+2) π -electrons. 2. Cyclizing condensation of 3,4-pyrroledicarboxaldehydes with compounds containing acidic CH and NH groups
 AU Kreher, Richard; Vogt, Guenther
 CS Inst. Org. Chem., Tech. Hochsch. Darmstadt, Darmstadt, Fed. Rep. Ger.
 SO Angewandte Chemie, International Edition in English (1970), 9(12), 955-6
 CODEN: ACIEAY; ISSN: 0570-0833
 DT Journal

LA English
 IT 30476-58-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 30476-58-5 CAPLUS
 CN 6H-Pyrrolo[3,4-d]pyridazine, 5,6,7-trimethyl- (8CI, 9CI) (CA INDEX NAME)



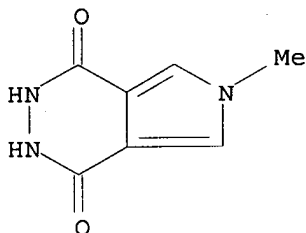
L9 ANSWER 18 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN
 TI Reactions of hydrazine with heterocyclic 1,2-dicarboxylic acid esters
 AB The appropriate dicarboxylic acid ester (0.1 mol) in 25-50 cc. MeOH treated with 15 g. N₂H₄.H₂O, kept several hrs. at room temperature, heated 0.5 h. on the steam bath, and evaporated, the residue dissolved in 50-500 cc. H₂O containing 5 cc. concentrated NH₄OH, the solution filtered and acidified with excess AcOH or HCl, and the crystalline precipitate washed and dried gave the following condensation products (m.p. and % yield given): 5,8-dihydroxy-1,4,6,7-tetrazanaphthalene (I), 280° (decomposition), 95; 1,3-dimethyl-5,8-dihydroxy-2,6,7-triazanaphthalene, 302° (decomposition), 97; 2-NH₂ derivative of I, above 400°, 93; 2-cyano-3-methyl-5,8-dihydroxy-4,6,7-triazanaphthalene, 320° (decomposition), 85; 2-cyano-3,8-dimethyl-5,8-dihydroxy-4,6,7-triazanaphthalene, 338-40°, 89; 1,4-dimethyl-5,8-dihydroxy-2,3,6,7-tetrazanaphthalene, 320° (decomposition), 73; 4,7-dihydroxy-2-thia-5,6-diazaindene, 328-30°, 92; 2-methyl-4,7-dihydroxy-1-thia-5,6-diazaindene, 294-5°, 90; 1-methyl-4,7-dihydroxy-2-oxa-5,6-diazaindene (II), 282-3°, 77; 3-Me derivative of II, 345° (decomposition), 83; 1-phenyl-2-methyl-4,7-dihydroxy-1,5,6-triazaindene, 335-7°, 89; 1-phenyl-4,7-dihydroxy-1,2,5,6-tetrazaindene, 315-16°, 61; 2-mercapto-4,7-dihydroxy-1,3,5,6-tetrazaindene (III), above 400°, 67; 1-methyl-4,7-dihydroxy-1,3,5,6-tetrazaindene, 354-6°, 78°; 1-Me derivative of III, above 330°, 93; 1-phenyl-4,7-dihydroxy-1,3,5,6-tetrazaindene (IV), 315-16°, 89°; 2-SH derivative of IV, 367° (decomposition), 97. The appropriate dicarboxylic dihydrazide (0.05 mol) refluxed 2-8 h. with 50 cc. N₂H₄.H₂O or heated 9-72 h. on the steam bath, the solution evaporated in vacuo on the steam bath, the solid residue dissolved in about 50-200 cc. hot H₂O, and the solution acidified with AcOH or HCl and cooled gave the following condensation products (m.p. and % yield given): 2-methyl-4,7-dihydroxy-1-oxa-5,6-diazaindene (V), 290-2°, 96; 4,7-dihydroxy-2,5,6-triazaindene (VI), above 310°, 90; 2-Me derivative (VII) of VI, 339-40°, 89; 1,5,6-isomer of V, 355° (decomposition), -; 4,7-dihydroxy-1,3,5,6-tetrazaindene (VIII), above 400°, 92. The appropriate dihydrazide (0.05 mol) in 100 cc. 2N HCl heated 6 h. on the steam bath, cooled, and filtered gave the following condensation products: 4,7-dihydroxy-2-oxa-5,6-diazaindene, above 300°, 70; V; VI; VII; VIII. The appropriate diester (0.1 mol) in about 50 cc. MeOH allowed to stand several hrs. with 15 g. N₂H₄.H₂O or heated 0.5 h. on the steam bath, and cooled, and the product recrystd. from H₂O or EtOH or dissolved in dilute acid and reprecipitated with NH₄OH gave the corresponding dicarboxylic acid dihydrazides (IX) of the following acids (m.p. and % yield of the IX given): 4,5-imidazoledicarboxylic acid, above 375°, 99; 3,4-pyrazoledicarboxylic acid, above 300°, 98;

3,4-furandicarboxylic acid (X), 270° (decomposition), 88;
 5-methyl-2,3-furandicarboxylic acid, m. 190°, 94;
 3,4-pyrroledicarboxylic acid (XI), above 300°, 95; 1-Me derivative of
 XI, 330° (decomposition), 90. Dihydrazide of X (16 g.) and 25 cc.
 N2H4.H2O heated 6 h. on the steam bath, the brown solution evaporated in vacuo,
 the residue dissolved in 100 cc. dilute aqueous NaOH, and the solution treated

with

C and acidified with AcOH gave 13 g. 3,3'-dihydroxy-4,4'-bipyrazole (XII),
 darkened at 360° but did not melt (from H2O); XII was also obtained
 in 50% yield from di-Et 1-formyl-2-diethoxymethylsuccinate in EtOH with
 excess N2H4. 1-Methyl-4,7-dihydroxy-2-oxa-5,6-diazaindene (XIII) (10 g.)
 heated 8 h. on the steam bath with 20 cc. N2H4.H2O gave 90% 5-Me derivative of
 XII, m. above 360° (sublimed at 275° and 0.1 mm.). The 3-Me
 derivative of XIII gave similarly the 5,5'-di-Me derivative of XII, m. above
 375°, in 52% yield when refluxed 15 h. with N2H4.

AN 1956:69457 CAPLUS <<LOGINID::20071212>>
 DN 50:69457
 OREF 50:13041a-h
 TI Reactions of hydrazine with heterocyclic 1,2-dicarboxylic acid esters
 AU Jones, Reuben G.
 CS Lilly Research Labs., Indianapolis, IN
 SO Journal of the American Chemical Society (1956), 78, 159-63
 CODEN: JACSAT; ISSN: 0002-7863
 DT Journal
 LA Unavailable
 OS CASREACT 50:69457
 IT 860362-71-6P, 6H-Pyrrolo[3,4-d]pyridazine-1,4-diol, 6-methyl-
 RL: PREP (Preparation)
 (preparation of)
 RN 860362-71-6 CAPLUS
 CN 6H-Pyrrolo[3,4-d]pyridazine-1,4-diol, 6-methyl- (5CI) (CA INDEX NAME)



=> d his

(FILE 'HOME' ENTERED AT 10:19:03 ON 12 DEC 2007)

FILE 'REGISTRY' ENTERED AT 10:19:12 ON 12 DEC 2007

L1 STRUCTURE UPLOADED
 L2 0 S L1
 L3 237 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 10:21:22 ON 12 DEC 2007

L4 7 S L3

FILE 'REGISTRY' ENTERED AT 10:28:45 ON 12 DEC 2007

L5 STRUCTURE UPLOADED
 L6 1 S L5
 L7 86 S L5 SSS FULL

FILE 'CAPLUS' ENTERED AT 10:29:37 ON 12 DEC 2007

L8 19 S L7
L9 18 S L8 NOT L4

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| FULL ESTIMATED COST | 112.21 | 478.25 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
| CA SUBSCRIBER PRICE | -16.38 | -21.84 |

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| CA SUBSCRIBER PRICE | -16.38 | -21.84 |

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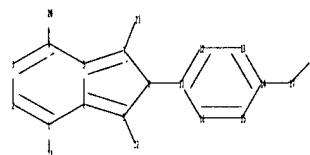
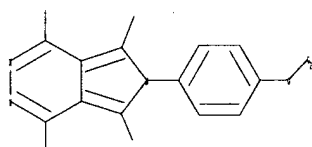
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chain nodes :

17 19 20 21 22 23

ring nodes :

1 2 3 4 5 6 7 8 9 11 12 13 14 15 16

chain bonds :

1-23 4-20 7-21 8-11 9-22 14-17 17-19

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 11-12 11-16 12-13 13-14 14-15
15-16

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 8-11 14-17 17-19

exact bonds :

1-23 4-20 7-21 9-22
normalized bonds :
11-12 11-16 12-13 13-14 14-15 15-16

G1:H,Cy

G2:H,CH3,Et,n-Pr,i-Pr,CF3

Match level :

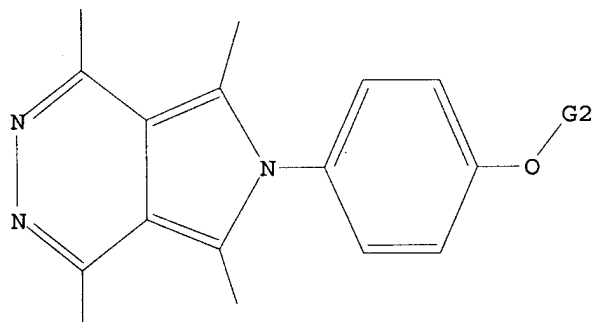
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22:CLASS 23:CLASS

L10 STRUCTURE UPLOADED

=> d l10

L10 HAS NO ANSWERS

L10 STR



G1 H,Cy

G2 H,Me,Et,n-Pr,i-Pr,CF3

Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SEARCH INITIATED 11:33:42 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 138 TO ITERATE

100.0% PROCESSED 138 ITERATIONS

3 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 2056 TO 3464

PROJECTED ANSWERS: 3 TO 163

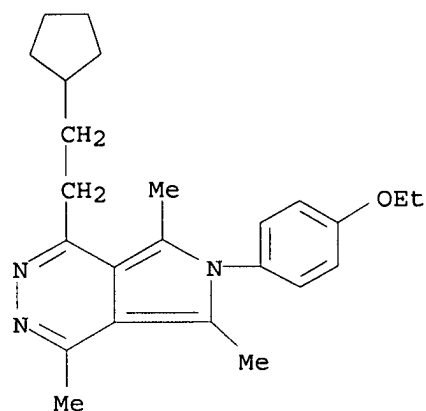
L11 3 SEA SSS SAM L10

=> d l11 scan

L11 3 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 6H-Pyrrolo[3,4-d]pyridazine, 1-(2-cyclopentylethyl)-6-(4-ethoxyphenyl)-
4,5,7-trimethyl-

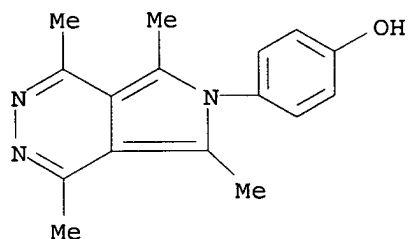
MF C24 H31 N3 O



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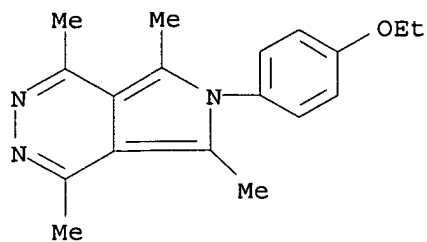
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L11 3 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Phenol, 4-(1,4,5,7-tetramethyl-6H-pyrrolo[3,4-d]pyridazin-6-yl)-
MF C16 H17 N3 O



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L11 3 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 6H-Pyrrolo[3,4-d]pyridazine, 6-(4-ethoxyphenyl)-1,4,5,7-tetramethyl-
MF C18 H21 N3 O



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> s l10 sss full

FULL SEARCH INITIATED 11:35:47 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 2820 TO ITERATE

100.0% PROCESSED 2820 ITERATIONS

54 ANSWERS

SEARCH TIME: 00.00.01

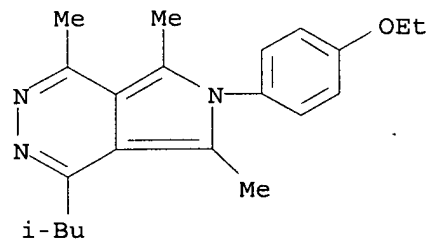
L12 54 SEA SSS FUL L10

=> d l12 scan

L12 54 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 6H-Pyrrolo[3,4-d]pyridazine, 6-(4-ethoxyphenyl)-1,5,7-trimethyl-4-(2-methylpropyl)-

MF C21 H27 N3 O



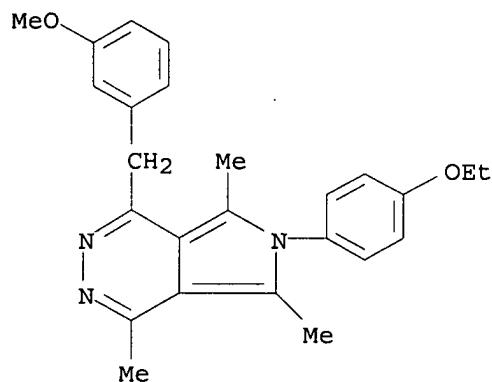
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HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L12 54 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

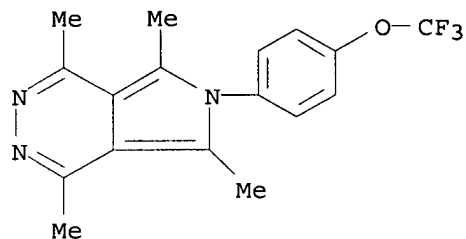
IN 6H-Pyrrolo[3,4-d]pyridazine, 6-(4-ethoxyphenyl)-1-[(3-methoxyphenyl)methyl]-4,5,7-trimethyl-

MF C25 H27 N3 O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L12 54 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
 IN 6H-Pyrrolo[3,4-d]pyridazine, 1,4,5,7-tetramethyl-6-[4-(trifluoromethoxy)phenyl]-
 MF C17 H16 F3 N3 O



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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| | ENTRY | SESSION |
| FULL ESTIMATED COST | 173.90 | 653.09 |
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| | ENTRY | SESSION |
| CA SUBSCRIBER PRICE | 0.00 | -21.84 |

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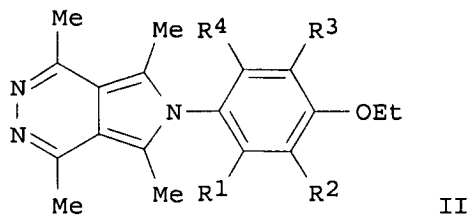
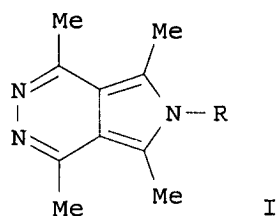
=> s l12

L13 4 L12

=> d l13 1-4 ti abs bib

L13 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN
TI Expedited SAR study of high-affinity ligands to the $\alpha 2\delta$ subunit of voltage-gated calcium channels: Generation of a focused library using a solution-phase Sn2Ar coupling methodology
AB The SAR of the lead compound 3, a novel ligand for the $\alpha 2\delta$ subunit of voltage-gated calcium channels, was rapidly explored. Utilizing a parallel solution-phase Sn2Ar coupling approach, a focused library was obtained. The library was evaluated in vitro and afforded a series of analogs with improved potencies. The SAR trends of the library are also described.
AN 2005:1342000 CAPLUS <<LOGINID::20071212>>
DN 144:100381
TI Expedited SAR study of high-affinity ligands to the $\alpha 2\delta$ subunit of voltage-gated calcium channels: Generation of a focused library using a solution-phase Sn2Ar coupling methodology
AU Chen, Chixu; Stearns, Brian; Hu, Tao; Anker, Naomi; Santini, Angelina; Arruda, Jeannie M.; Campbell, Brian T.; Datta, Purabi; Aiyar, Jayashree; Munoz, Benitio
CS Department of Chemistry, Merck Research Laboratories, San Diego, CA, 92121, USA
SO Bioorganic & Medicinal Chemistry Letters (2006), 16(3), 746-749
CODEN: BMCLE8; ISSN: 0960-894X
PB Elsevier B.V.
DT Journal
LA English
OS CASREACT 144:100381
RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN
TI Synthesis and biological evaluation of 6-aryl-6H-pyrrolo[3,4-d]pyridazine derivatives as high-affinity ligands of the $\alpha 2\delta$ subunit of voltage-gated calcium channels
GI



AB 2H-pyrrolo[3,4-c]pyridazines I (R = 4-EtOC₆H₄, 2-EtO-5-pyridinyl, 5-EtO-2-pyridinyl, 5-EtO-2-pyrazinyl, 4-EtO-1-pyridazinyl, 2-EtO-5-pyrimidinyl, etc.) such as II (R₁ = H, MeO, Et, H₂C:CH, Me, MeS, EtO, F; R₂ = H, Me; R₃ = H, Me, Cl, HOCH₂; R₄ = H, Me) are prepared as ligands for the α 2 δ subunit of voltage-gated calcium channels. Ortho-substituents capable of electron-donation increase the binding of II to the α 2 δ subunit of voltage-gated calcium channels; electron-withdrawing substituents in the ortho-position of II decrease binding significantly. II (R₁ = MeO; R₂ = R₃ = R₄ = H) binds to the α 2 δ subunit of voltage-gated calcium channels from A710 cells with an IC₅₀ value of 4 nM. Testing of tritiated ligand II (R₁ = TCH₂TCH; R₂ = R₃ = R₄ = H) in purified human α 2 δ voltage-gated calcium channel subunits indicates that II displace Gabapentin from the α 2 δ subunit of voltage-gated calcium channels, and thus act as Gabapentin mimics in vitro. In the preparation of II (R₁ = Et; R₂ = R₃ = R₄ = H), a novel metal-free hydrogenation is used using hydrazine as the reductant; the reduction is effective in other systems (no data).

AN 2004:303255 CAPLUS <<LOGINID::20071212>>

DN 141:54277

TI Synthesis and biological evaluation of 6-aryl-6H-pyrrolo[3,4-d]pyridazine derivatives as high-affinity ligands of the α 2 δ subunit of voltage-gated calcium channels

AU Hu, Tao; Stearns, Brian A.; Campbell, Brian T.; Arruda, Jeannie M.; Chen, Chixu; Aiyar, Jayashree; Bezverkov, Robert E.; Santini, Angelina; Schaffhauser, Herve; Liu, Wensheng; Venkatraman, Shankar; Munoz, Benito

CS MRLSDB2, Department of Medicinal Chemistry, Merck Research Laboratories, San Diego, CA, 92121, USA

SO Bioorganic & Medicinal Chemistry Letters (2004), 14(9), 2031-2034
CODEN: BMCLE8; ISSN: 0960-894X

PB Elsevier Science B.V.

DT Journal

LA English

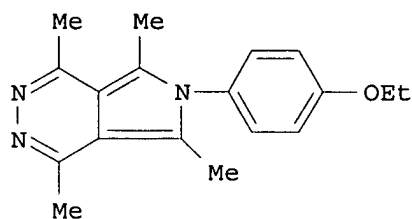
OS CASREACT 141:54277

RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN

TI Synthesis and biological evaluation of 6-aryl-6H-pyrrolo[3,4-d]pyridazine derivatives: high-affinity ligands to the α 2 δ subunit of voltage gated calcium channels

GI



I

AB A novel class of 6-aryl-6H-pyrrolo[3,4-d]pyridazine ligands for the $\alpha 2\delta$ subunit of voltage-gated calcium channels has been described. Substitutions in the aryl ring of the mol. were generally not tolerated, and resulted in diminished binding to the $\alpha 2\delta$ subunit. Modifications to the pyridazine ring revealed numerous permissive substitutions, and detailed SAR studies were carried out in this portion of the mol. Replacement of the pyridazine ring Me group with an aminomethyl functionality provided greatly improved potency over the initial lead. The initial lead compound (I) displayed good rat pharmacokinetic properties, and was shown to be efficacious in the Chung model for neuropathic pain in rats.

AN 2004:153601 CAPLUS <<LOGINID::20071212>>

DN 140:357282

TI Synthesis and biological evaluation of 6-aryl-6H-pyrrolo[3,4-d]pyridazine derivatives: high-affinity ligands to the $\alpha 2\delta$ subunit of voltage gated calcium channels

AU Stearns, Brian A.; Anker, Naomi; Arruda, Jeannie M.; Campbell, Brian T.; Chen, Chixu; Cramer, Merryl; Hu, Tao; Jiang, Xiaohui; Park, Kenneth; Ren, Kun Kun; Sablad, Marciano; Santini, Angelina; Schaffhauser, Herve; Urban, Mark O.; Munoz, Benito

CS Department of Medicinal Chemistry, Merck Research Laboratories, San Diego, CA, 92121, USA

SO Bioorganic & Medicinal Chemistry Letters (2004), 14(5), 1295-1298
CODEN: BMCLE8; ISSN: 0960-894X

PB Elsevier Science B.V.

DT Journal

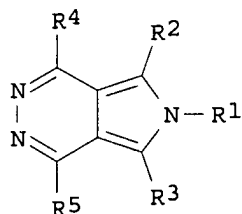
LA English

OS CASREACT 140:357282

RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN

TI Treatment of neuropathic pain with 6H-pyrrolo[3,4-d]pyridazine compounds
GI



I

AB The title compds. [I; R1 = (un)substituted alkyl(hetero)aryl, alkyl(hetero)cycloalkyl, (hetero)aryl, (hetero)cycloalkyl; R2-R5 = a bond, (un)substituted alkyl, alkyl(hetero)aryl, alkyl(hetero)cycloalkyl, (hetero)aryl, (hetero)cycloalkyl] were prepared as as ligands of voltage

gated calcium channels (VGCC), useful in the treatment of neuropathic pain, and psychiatric and mood disorders such as, for example, schizophrenia, anxiety, depression, panic, and bipolar disorder, as well as in the treatment of pain, Parkinson s disease, cognitive dysfunction, epilepsy, circadian rhythm disorders, drug addiction, drug abuse, drug withdrawal and other. E.g., a multi-step synthesis of I [R1 = 4-EtOC6H4; R2-R4 = Me; R5 = 4-MeOC6H4] which produced a 65% effect after i.p. dosing at 30 mg/kg in spinal nerve ligation model of neuropathic pain in rats, was given. The pharmaceutical composition comprising the compound I is

claimed.

AN 2004:60243 CAPLUS <<LOGINID::20071212>>

DN 140:111422

TI Treatment of neuropathic pain with 6H-pyrrolo[3,4-d]pyridazine compounds

IN Anker, Naomi Burke; Arruda, Jeannie M.; Campbell, Brian Thomas; Munoz, Benito; Prasit, Petpiboon; Stearns, Brian A.

PA Merck & Co., Inc., USA

SO PCT Int. Appl., 203 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
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| PI | WO 2004006836 | A2 | 20040122 | WO 2003-US21493 | 20030708 |
| | WO 2004006836 | A3 | 20040415 | | |
| | W: | | | | |
| | AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
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| | EP 1539168 | A2 | 20050615 | EP 2003-764414 | 20030708 |
| | R: | | | | |
| | AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK | | | | |
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| OS | MARPAT 140:111422 | | | | |